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=> fil reg; d stat que l19; fil capl; d que nos 123
FILE 'REGISTRY' ENTERED AT 09:44:18 ON 29 JUN 2007
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STRUCTURE FILE UPDATES:   28 JUN 2007  HIGHEST RN 940062-32-8
DICTIONARY FILE UPDATES:  28 JUN 2007  HIGHEST RN 940062-32-8

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

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experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

L3                STR
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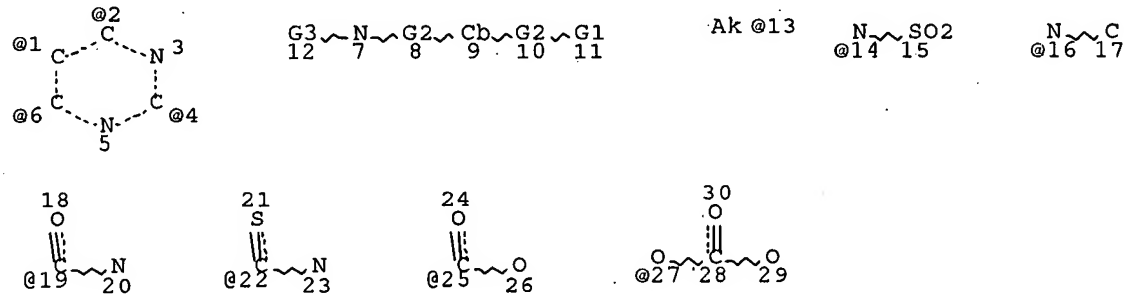


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CONNECT IS E2  RC AT   9
CONNECT IS E2  RC AT  13
DEFAULT MLEVEL IS ATOM
GGCAT    IS MCY  SAT  AT   9
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ECOUNT   IS M4-X7 C  AT   9

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS  30
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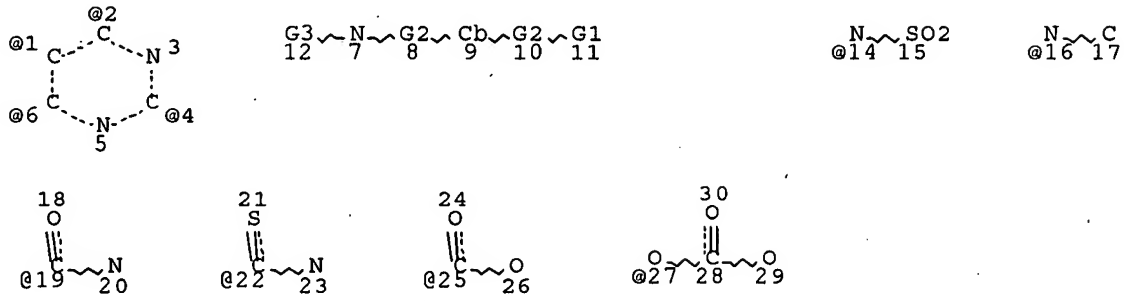
STEREO ATTRIBUTES: NONE
L9 563914 SEA FILE=REGISTRY ABB=ON 46.195.39/RID
L16 STR



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CONNECT IS E2 RC AT 9
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DEFAULT ECLEVEL IS LIMITED
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GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE
L19 3163 SEA FILE=REGISTRY SUB=L9 SSS FUL (L16 AND L3)

100.0% PROCESSED 563914 ITERATIONS 3163 ANSWERS
SEARCH TIME: 00.00.11

FILE 'CAPLUS' ENTERED AT 09:44:18 ON 29 JUN 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 29 Jun 2007 VOL 147 ISS 2
FILE LAST UPDATED: 28 Jun 2007 (20070628/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

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L3              STR
L9       563914 SEA FILE=REGISTRY ABB=ON  46.195.39/RID
L16             STR
L19        3163 SEA FILE=REGISTRY SUB=L9 SSS FUL (L16 AND L3)
L22          77 SEA FILE=CAPLUS ABB=ON  L19
L23          39 SEA FILE=CAPLUS ABB=ON  L22 AND (PY<2003 OR AY<2003 OR
                PRY<2003)
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=> d ibib ed abs hitstr 123 1-39; fil hom

L23 ANSWER 1 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:857175 CAPLUS Full-text
DOCUMENT NUMBER: 141:350167
TITLE: Preparation of imidazolin-2-one derivatives as p38 MAP kinase inhibitors
INVENTOR(S): Kubo, Akira; Imashiro, Ritsuo; Sakurai, Hiroaki; Miyoshi, Hidetaka; Ogasawara, Akihito; Hiramatsu, Hajime; Nakajima, Tatsuo; Nakane, Tetsu
PATENT ASSIGNEE(S): Japan
SOURCE: U.S. Pat. Appl. Publ., 76 pp., Cont.-in-part of Appl. No. PCT/JP02/10937.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004204426	A1	20041014	US 2004-827294	20040420 <--
WO 2003035638	A1	20030501	WO 2002-JP10937	20021022 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004201666	A1	20040513	AU 2004-201666	20040421 <--
WO 2004094404	A1	20041104	WO 2004-JP5716	20040421
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SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

JP 2004339210	A	20041202	JP 2004-125060	20040421
EP 1628968	A1	20060301	EP 2004-728708	20040421

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK

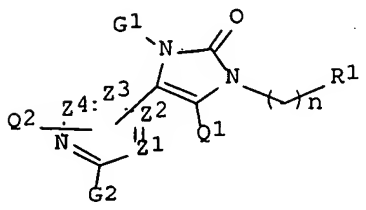
PRIORITY APPLN. INFO.:

JP 2001-324029	A	20011022 <--
JP 2002-263680	A	20020910 <--
WO 2002-JP210937	A2	20021022 <--
JP 2003-116076	A	20030421
AU 2002-363108	A3	20021022 <--
WO 2004-JP5716	W	20040421

OTHER SOURCE(S): MARPAT 141:350167

ED Entered STN: 18 Oct 2004

GI



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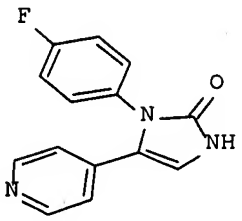


II

AB The title compds. I [wherein G1 = (un)substituted alkyl or B-W; B = (un)substituted Ph, naphthyl, aromatic heterocyclyl, or cycloalkyl; W = a single bond or (un)substituted alkylene; Q1 and Q2 = independently H, halo, alkyl; n = 0-4; R1 = H, (un)substituted (cyclo)alkyl, Ph, or heterocyclyl; Z1-Z4 = independently CH or N with exclusions; G2 = H, NR3R4, OR5, SR5, COR6, CHR7R8, or heterocyclyl; R3-R8 = independently H, alkenyl, alkynyl, OH, alkoxy, alkoxyoxalyl, alkylsulfonyl, (un)substituted alkyl, amino, alkanoyl, carbamoyl, cycloalkyl, Ph, heterocyclyl(carbonyl), PhCO, or heterocyclyl-CO] and pharmaceutically acceptable salts were prepared as p38 mitogen activation proteins (MAP) kinase inhibitors. Thus, reacting 2,2-diethoxy-2-(pyridin-4-yl)ethylamine (preparation given) with 4-fluorophenyl isocyanate afforded the imidazolinone II. The representative compds. I significantly reduced the production of TNF-α in mice in vivo.

IT 521090-75-5P 521090-76-6P 521091-56-5P
521091-59-8P 521091-62-3P 521091-63-4P
521091-65-6P

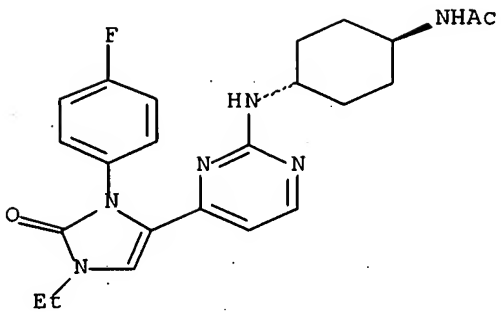
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(MAP kinase inhibitor; preparation of imidazolinones as p38 MAP kinase inhibitors)

RN 521090-75-5 CAPLUS

CN Acetamide, N-[trans-4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

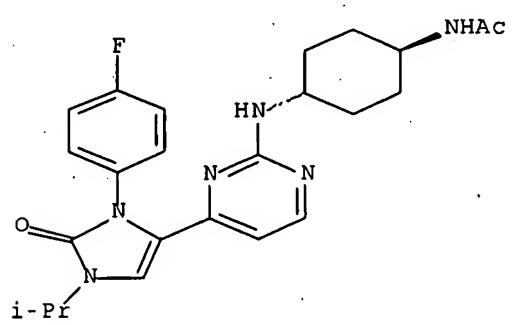
Relative stereochemistry.



● HCl

RN 521090-76-6 CAPLUS
CN Acetamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(1-methylethyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

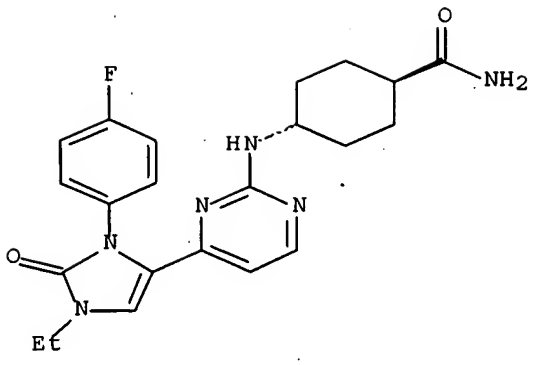
Relative stereochemistry.



● HCl

RN 521091-56-5 CAPLUS
CN Cyclohexanecarboxamide, 4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]-, monohydrochloride, trans- (9CI) (CA INDEX NAME)

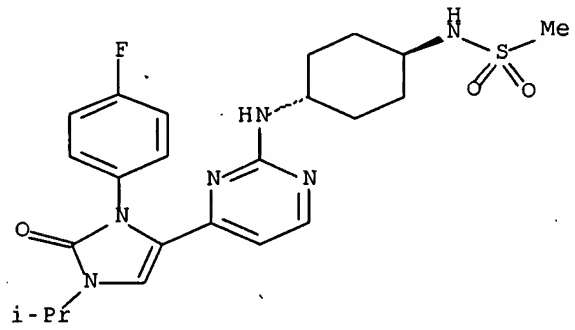
Relative stereochemistry.



● HCl

RN 521091-59-8 CAPLUS
CN Methanesulfonamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(1-methylethyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

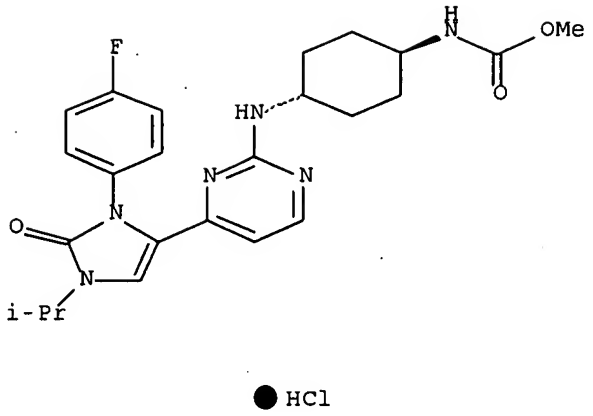
Relative stereochemistry.



● HCl

RN 521091-62-3 CAPLUS
CN Carbamic acid, [trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(1-methylethyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

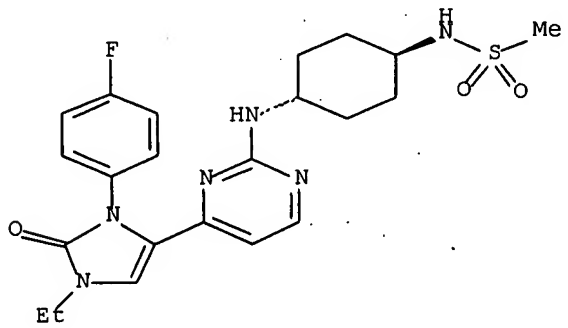
Relative stereochemistry.



● HCl

RN 521091-63-4 CAPLUS
CN Methanesulfonamide, N-[trans-4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

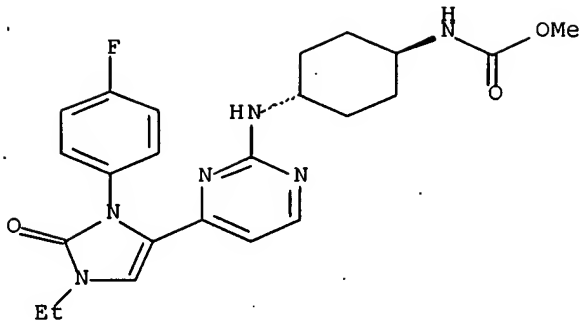
Relative stereochemistry.



● HCl

RN 521091-65-6 CAPLUS
CN Carbamic acid, [trans-4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



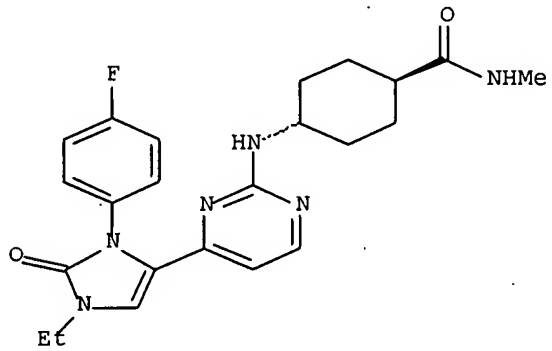
● HCl

IT 774579-17-8P 774580-02-8P 774580-12-0P
774580-20-0P 774580-26-6P 774580-27-7P
774580-28-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of imidazolinones as p38 MAP kinase inhibitors)

RN 774579-17-8 CAPLUS

CN Cyclohexanecarboxamide, 4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]-N-methyl-, monohydrochloride, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

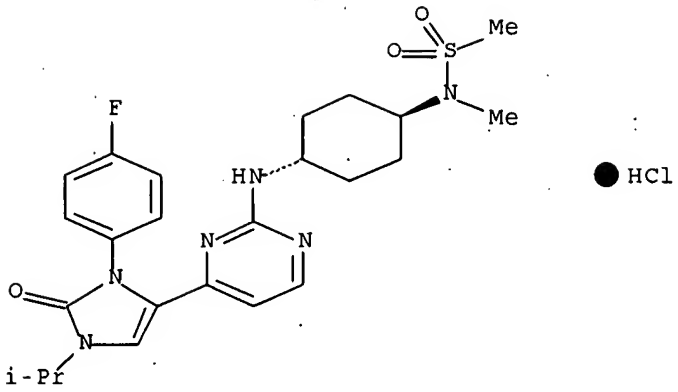


● HCl

RN 774580-02-8 CAPLUS

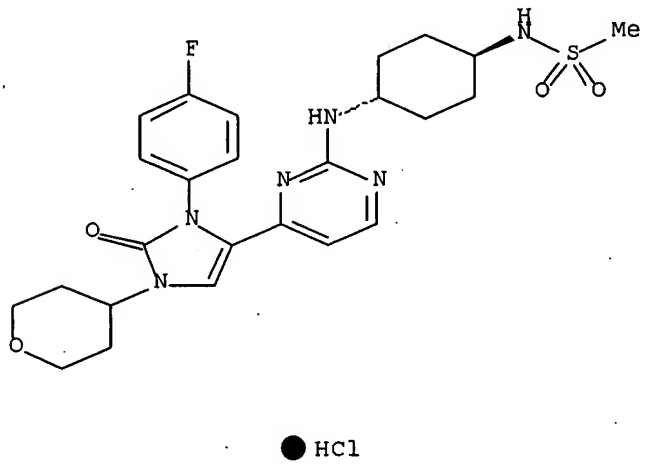
CN Methanesulfonamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(1-methylethyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 774580-12-0 CAPLUS
CN Methanesulfonamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1-(tetrahydro-2H-pyran-4-yl)-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



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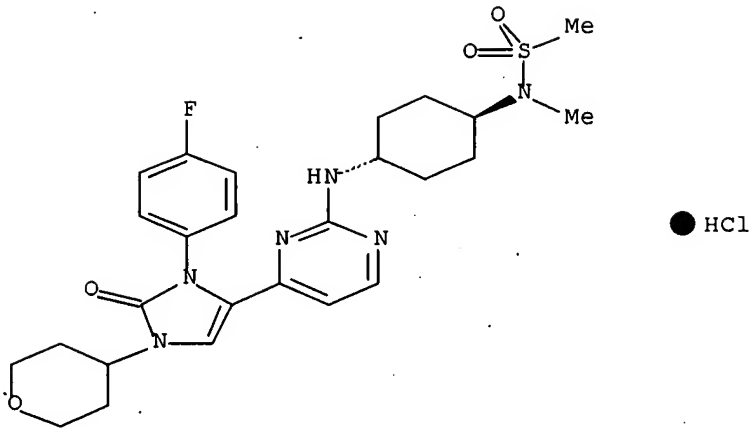
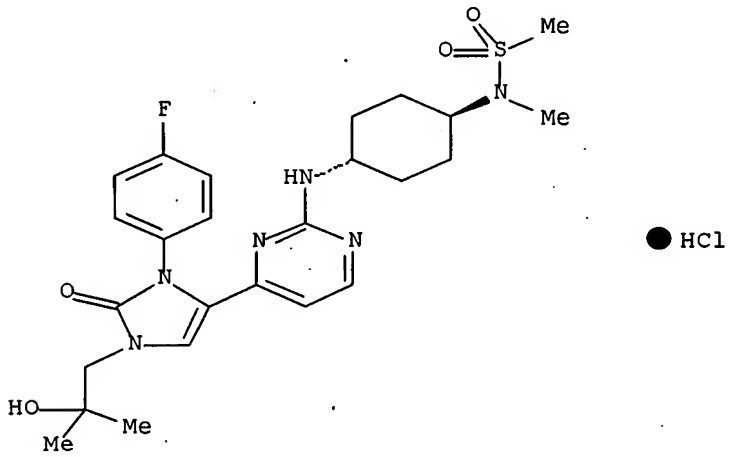
CN Methanesulfonamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1-(tetrahydro-2H-pyran-4-yl)-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



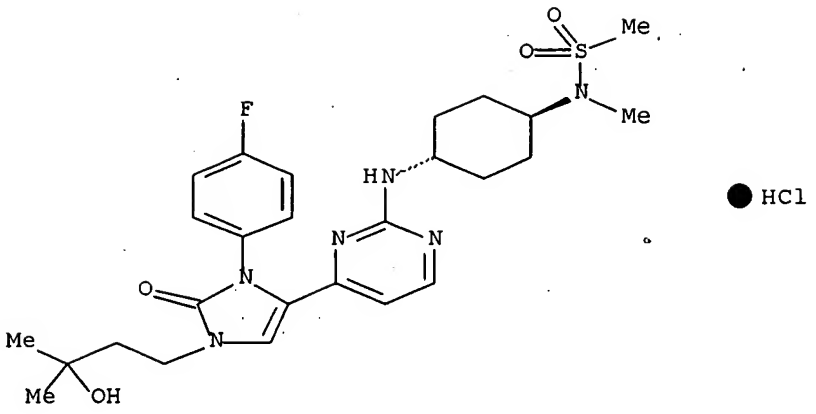
RN 774580-26-6 CAPLUS
CN Methanesulfonamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(2-hydroxy-2-methylpropyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



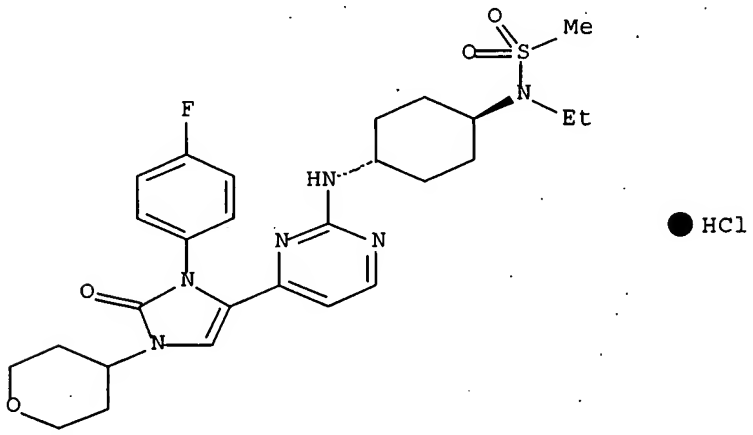
RN 774580-27-7 CAPLUS
CN Methanesulfonamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(3-hydroxy-3-methylbutyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 774580-28-8 CAPLUS
CN Methanesulfonamide, N-ethyl-N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1-(tetrahydro-2H-pyran-4-yl)-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



L23 ANSWER 2 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:588212 CAPLUS Full-text
DOCUMENT NUMBER: 141:140458
TITLE: Preparation of imidazopyrimidines as tyrosine kinase inhibitors
INVENTOR(S): Hirabayashi, Akihito; Mukoyama, Harunobu; Shiohara, Hiroaki; Kobayashi, Hiroaki; Terao, Yoshihiro; Miyazawa, Keiji; Misawa, Keiko; Onoda, Hideki
PATENT ASSIGNEE(S): Kissei Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 117 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

JP 2004203748	A	20040722	JP 2002-371196	20021224 <--
PRIORITY APPLN. INFO.:			JP 2002-371196	20021224 <--

OTHER SOURCE(S): MARPAT 141:140458
ED Entered STN: 23 Jul 2004
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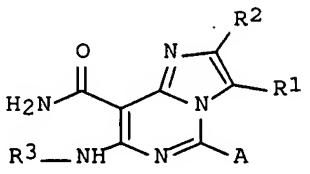

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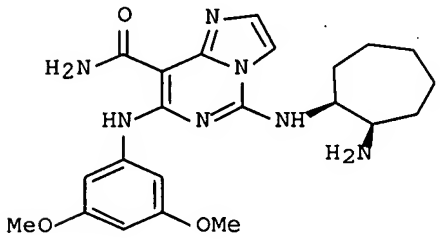


II

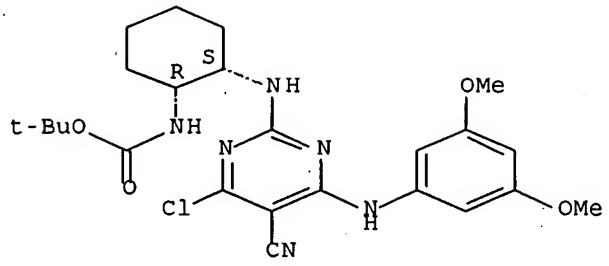
AB Title compds. I [R1, R2 = H, alkyl, etc.; R3 = H, alkyl, etc.; A = H, alkyl, etc.] were disclosed. In Syk tyrosine kinase inhibition assays, the Ki value of compound II was 1.6 nM. Of note, compds. I have potent inhibition activity against ZAP-70 and/or Syk tyrosine kinase. Compds. I are claimed useful for the treatment of bronchial asthma, allergic rhinitis, etc.

IT 725238-07-3P 725238-09-5P 725238-13-1P
725238-14-2P 725238-15-3P 725238-16-4P
725238-17-5P 725238-18-6P 725238-19-7P
725238-20-0P 725238-21-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of imidazopyrimidines as tyrosine kinase inhibitors for treatment of bronchial asthma and allergic dermatitis)

RN 725238-07-3 CAPLUS

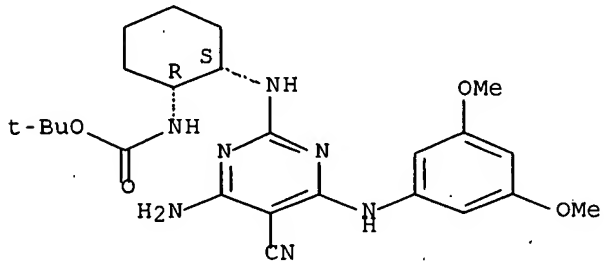
CN Carbamic acid, [(1R,2S)-2-[[4-chloro-5-cyano-6-[(3,5-dimethoxyphenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



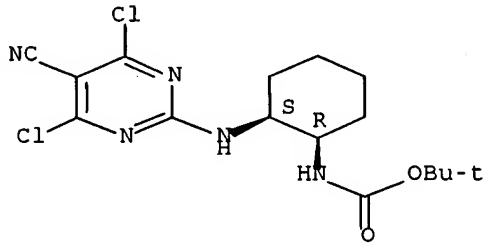
RN 725238-09-5 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[4-amino-5-cyano-6-[(3,5-dimethoxyphenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



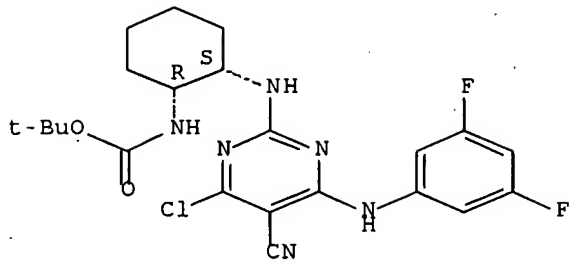
RN 725238-13-1 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[(4,6-dichloro-5-cyano-2-pyrimidinyl)amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



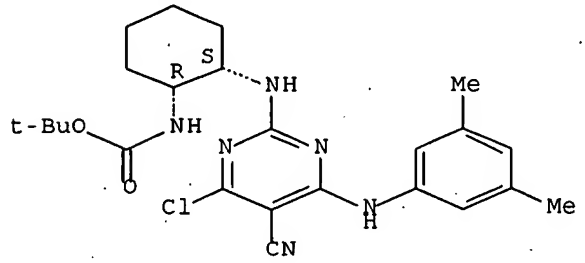
RN 725238-14-2 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[4-chloro-5-cyano-6-[(3,5-difluorophenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



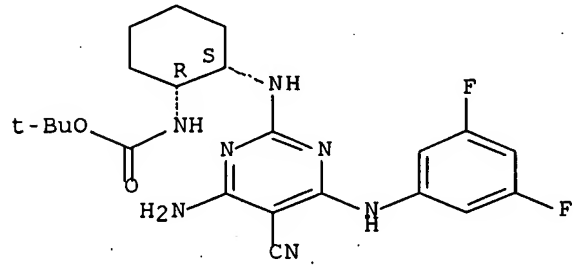
RN 725238-15-3 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[4-chloro-5-cyano-6-[(3,5-dimethylphenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



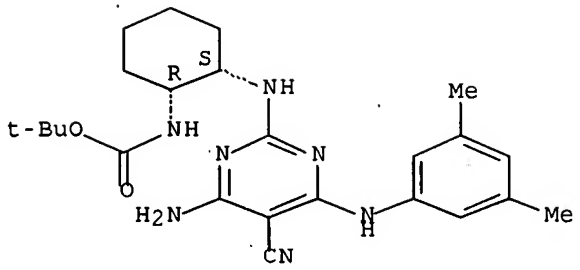
RN 725238-16-4 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[4-amino-5-cyano-6-[(3,5-difluorophenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



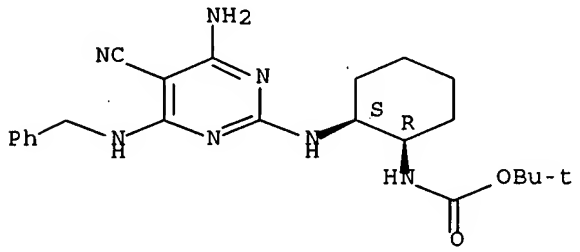
RN 725238-17-5 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[4-amino-5-cyano-6-[(3,5-dimethylphenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



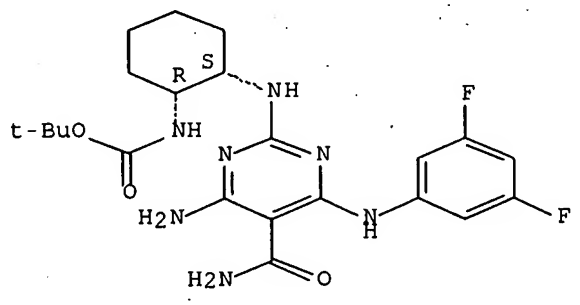
RN 725238-18-6 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[4-amino-5-cyano-6-[(phenylmethyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



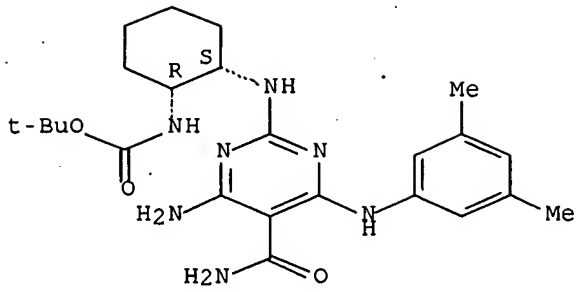
RN 725238-19-7 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[4-amino-5-(aminocarbonyl)-6-[(3,5-difluorophenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



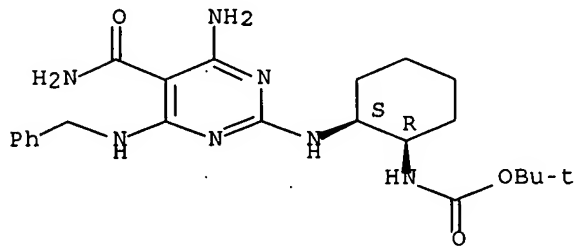
RN 725238-20-0 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[4-amino-5-(aminocarbonyl)-6-[(3,5-dimethylphenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 725238-21-1 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[4-amino-5-(aminocarbonyl)-6-[(phenylmethyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L23 ANSWER 3 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:142963 CAPLUS Full-text
DOCUMENT NUMBER: 140:199334
TITLE: Preparation of 2,4-pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of autoimmune diseases
INVENTOR(S): Singh, Rajinder; Argade, Ankush; Payan, Donald G.; Clough, Jeffrey; Keim, Holger; Sylvain, Catherine; Li, Hui; Bhamidipati, Somasekhar
PATENT ASSIGNEE(S): Rigel Pharmaceuticals, USA
SOURCE: PCT Int. Appl., 811 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004014382	A1	20040219	WO 2003-US24087	20030729 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,

	KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2492325		A1	20040219	CA 2003-2492325	20030729 <--
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BR 2003013059		A	20050705	BR 2003-13059	20030729 <--
CN 1678321		A	20051005	CN 2003-821120	20030729 <--
JP 2006514989		T	20060518	JP 2005-506142	20030729 <--
NZ 537752		A	20061222	NZ 2003-537752	20030729 <--
US 2007060603		A1	20070315	US 2003-631029	20030729 <--
US 2005038243		A1	20050217	US 2004-858343	20040601 <--
US 7060827		B2	20060613		
US 2005209230		A1	20050922	US 2004-911684	20040803 <--
SE 2005000203		A	20050329	SE 2005-203	20050127 <--
NO 2005001069		A	20050228	NO 2005-1069	20050228 <--
IN 2005KN00302		A	20060421	IN 2005-KN302	20050228 <--
US 2006025410		A1	20060202	US 2005-149105	20050608 <--
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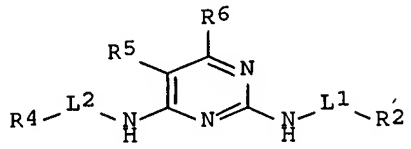
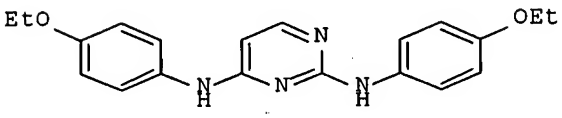
US 2006058292		A1	20060316	US 2005-149418	20050608 <--
US 2006135543		A1	20060622	US 2005-299207	20051208 <--
PRIORITY APPLN. INFO.:				US 2002-399673P	P 20020729 <--
				US 2003-443949P	P 20030131
				US 2003-452339P	P 20030306
				US 2003-631029	A 20030729
				US 2002-353267P	P 20020201 <--
				US 2002-353333P	P 20020201 <--
				US 2002-434277P	P 20021217 <--
				US 2003-355543	A1 20030131
				WO 2003-US24087	W 20030729
				US 2004-858343	A3 20040601

OTHER SOURCE(S): MARPAT 140:199334
ED Entered STN: 22 Feb 2004
GI



I



II

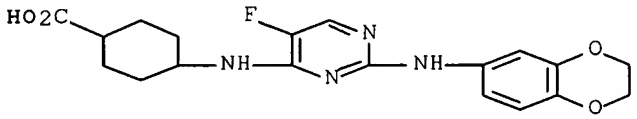
AB The present invention provides methods of treating or preventing autoimmune diseases with 2,4-pyrimidinediamine compds., as well as methods of treating, preventing or ameliorating symptoms associated with such diseases. Title compds. I [wherein L1 and L2 = independently a bond or a linker; R2 = (un)substituted alkyl, (hetero)cycloalkyl, or (hetero)aryl; R4 = H or R2; R5 =

R6 or (un)substituted alkyl, alkenyl, or alkynyl; R6 = independently H, an electroneg. group, protected alc. or thiol, haloalkyl(oxy), halo, CN, NC, OCN, SCN, NO, NO2, N3, or (un)substituted amino, sulfamoyl(oxy), acyl, carboxy, carbamoyl, (hetero)aryl(alkyl), etc.; with provisos and exclusions; and salts, hydrates, solvates, N-oxides, and prodrugs thereof] were prepared as inhibitors of the IgE and/or IgG receptor signaling cascades that lead to the release of chemical mediators. For example, coupling of 2,4-dichloropyrimidine with 4-ethoxyaniline in EtOH provided N2,N4-bis(4-ethoxyphenyl)-2,4- pyrimidinediamine (II). The latter inhibited degranulation of bone marrow derived mast cells challenged with anti-IgE and ionomycin with IC50 values of 4.5 μM and 4.4 μM, resp. Thus, I and their pharmaceutical compns. are useful in the treatment and prevention of diseases characterized by, caused by, or associated with the release of chemical mediators via degranulation of mast, basophil, neutrophil, or eosinophil cells and other processes effected by activation of the IgE and/or IgG receptor signaling cascades. Specific examples of autoimmune diseases that can be treated or prevented with I and their pharmaceutical compns. include rheumatoid arthritis, systemic lupus erythematosis, and multiple sclerosis (no data).

IT 575476-86-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(IgE and/or IgG receptor modulator; preparation of pyrimidinediamines as IgE
and/or IgG receptor modulators for treatment of autoimmune diseases)

RN 575476-86-7 CAPLUS

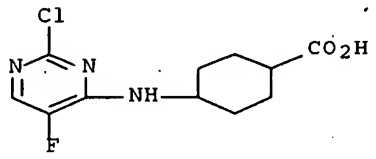
CN Cyclohexanecarboxylic acid, 4-[[2-[(2,3-dihydro-1,4-benzodioxin-6-yl)amino]-5-fluoro-4-pyrimidinyl]amino]- (CA INDEX NAME)



IT 575476-87-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for
treatment of autoimmune diseases)

RN 575476-87-8 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[(2-chloro-5-fluoro-4-pyrimidinyl)amino]- (9CI) (CA INDEX NAME)



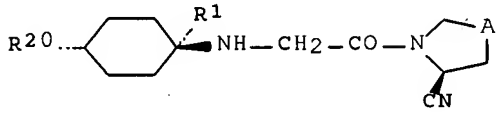
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 4 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:17853 CAPLUS Full-text
DOCUMENT NUMBER: 140:71039
TITLE: Pharmaceutical compositions containing aliphatic group-containing five-membered nitrogen heterocyclic compounds
INVENTOR(S): Yasuda, Kosuke; Morimoto, Keiji; Kanan, Saburo; Hikota, Masaki; Matsumoto, Takeshi; Arakawa, Kenji
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 83 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 2004002368	A	20040108	JP 2003-101362		20030404 <--
PRIORITY APPLN. INFO.:			JP 2002-102758	A	20020404 <--

OTHER SOURCE(S): MARPAT 140:71039
ED Entered STN: 09 Jan 2004
GI



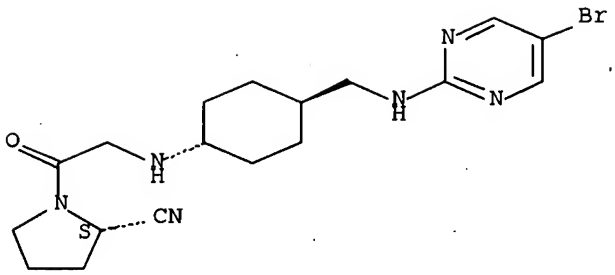
I

AB Pharmaceutical compns., which inhibit dipeptidyl peptidase IV (DPPIV) and are especially useful for prevention or treatment of type 2 diabetes, contain aliphatic group-containing 5-membered N heterocyclic compds. I [A = CH2, S; R1 = H, lower (hydroxy)alkyl, lower alkoxy-lower alkyl; R20 = (substituted) monocyclic or bicyclic heterocyclyl] or their pharmacol. acceptable salts as active ingredients. I-2HCl (R1 = H, R20 = phthalimido) (preparation given) inhibited DPPIV in human serum with IC50 of 3.8 nM.

IT 412355-56-7P 412355-59-0P 412355-60-3P
412355-61-4P 412355-75-0P 412355-76-1P
412355-77-2P 412355-78-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aliphatic group-containing five-membered nitrogen heterocyclic
compds. as dipeptidyl peptidase IV inhibitors for treatment of diabetes, etc.)

RN 412355-56-7 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[(5-bromo-2-pyrimidinyl)amino]methyl]cyclohexyl]amino]acetyl]-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

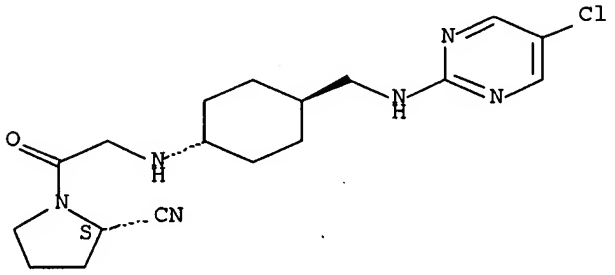
Absolute stereochemistry.



● HCl

RN 412355-59-0 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[(5-chloro-2-pyrimidinyl)amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI) (CA INDEX NAME)

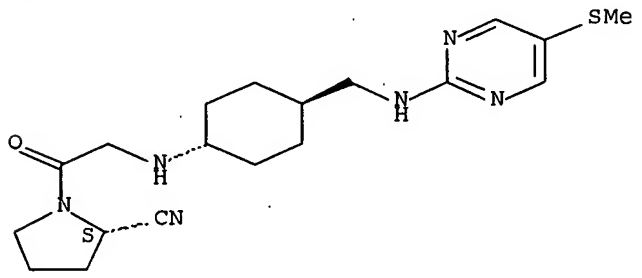
Absolute stereochemistry.



●2 HCl

RN 412355-60-3 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[[5-(methylthio)-2-pyrimidinyl]amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI) (CA INDEX NAME)

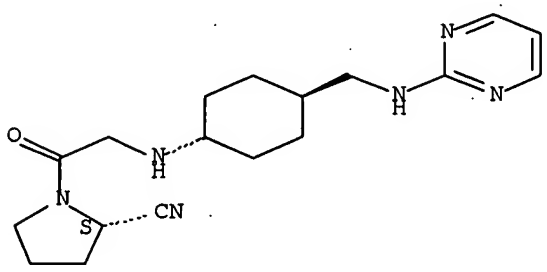
Absolute stereochemistry.



●2 HCl

RN 412355-61-4 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(2-pyrimidinylamino)methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

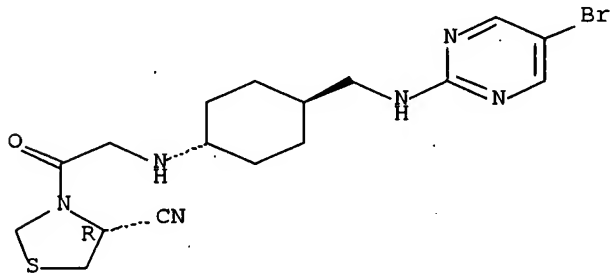
Absolute stereochemistry.



●2 HCl

RN 412355-75-0 CAPLUS
CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[[(5-bromo-2-pyrimidinyl)amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

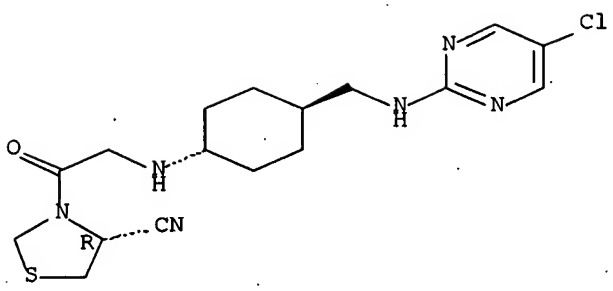
Absolute stereochemistry.



●2 HCl

RN 412355-76-1 CAPLUS
CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[[(5-chloro-2-pyrimidinyl)amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

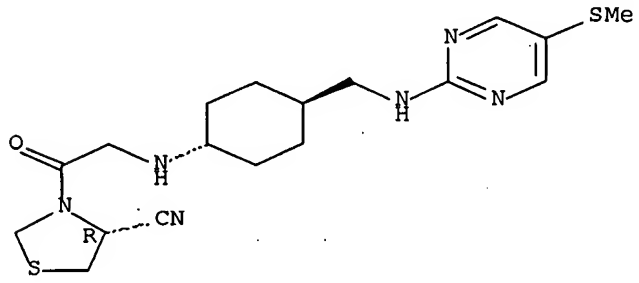
Absolute stereochemistry.



●2 HCl

RN 412355-77-2 CAPLUS
CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[[[5-(methylthio)-2-pyrimidinyl]amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

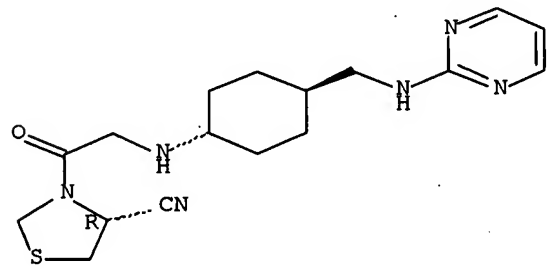
Absolute stereochemistry.



●2 HCl

RN 412355-78-3 CAPLUS
CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[(2-pyrimidinylamino)methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

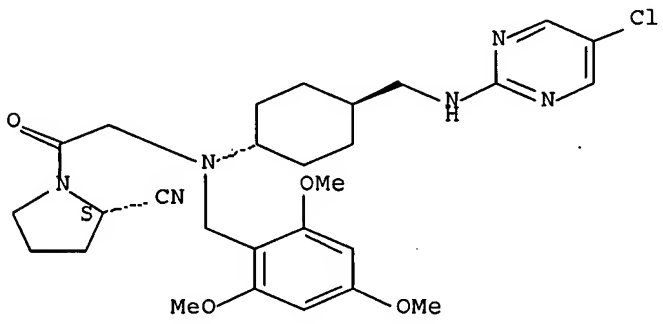
Absolute stereochemistry.



●2 HCl

IT 412357-18-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aliphatic group-containing five-membered nitrogen heterocyclic compds. as dipeptidyl peptidase IV inhibitors for treatment of diabetes, etc.)
RN 412357-18-7 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[(5-chloro-2-pyrimidinyl)amino]methyl]cyclohexyl][(2,4,6-trimethoxyphenyl)methyl]amino]acetyl]-, (2S)- (9CI) (CA INDEX NAME)

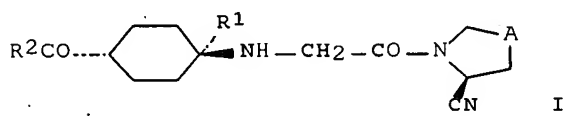
Absolute stereochemistry.



L23 ANSWER 5 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:17852 CAPLUS Full-text
DOCUMENT NUMBER: 140:71038
TITLE: Pharmaceutical compositions containing aliphatic N-containing 5-membered compounds as dipeptidylpeptidase IV (DPPIV) inhibitors
INVENTOR(S): Yasuda, Kosuke; Morimoto, Keiji; Kanan, Saburo; Hikota, Masaki; Matsumoto, Takeshi; Arakawa, Kenji
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 129 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 2004002367	A	20040108	JP 2003-101361		20030404 <--
PRIORITY APPLN. INFO.:			JP 2002-102757	A	20020404 <--

OTHER SOURCE(S): MARPAT 140:71038
ED Entered STN: 09 Jan 2004
GI



I

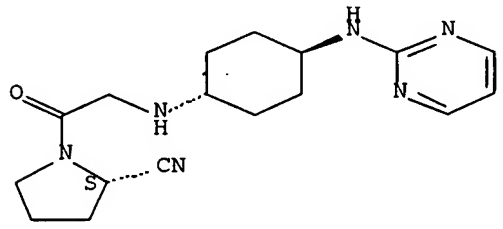
AB The compns., useful for prevention and treatment of type 2 diabetes, contain the compds. I [A = CH2, S; R1 = H, lower alkyl, hydroxyalkyl, alkoxyalkyl; R2 = (un)substituted mono-, di-, or tricyclic hydrocarbyl, heterocyclyl, (un)substituted amino] or their salts. I.HCl (A = CH2, R1 = H, R2 = NMe2) in vitro inhibited human blood serum DPPIV with IC50 of 3 nM.

IT 412284-89-0P 412284-90-3P 412284-91-4P
412284-92-5P 412285-02-0P 412285-03-1P
412285-05-3P 412285-08-6P 412285-09-7P
412285-11-1P 412285-12-2P 412285-13-3P
412285-14-4P 412285-15-5P 412285-16-6P
412285-17-7P 412285-18-8P 412285-19-9P
412285-20-2P 412285-21-3P 412285-22-4P
412285-43-9P 412285-44-0P 412285-45-1P
412285-64-4P 412285-65-5P 412288-75-6P
412288-76-7P 412288-77-8P 412288-78-9P
412915-48-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aliphatic N-containing 5-membered compds. as dipeptidylpeptidase IV
inhibitors)

RN 412284-89-0 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-(2-pyrimidinylamino)cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

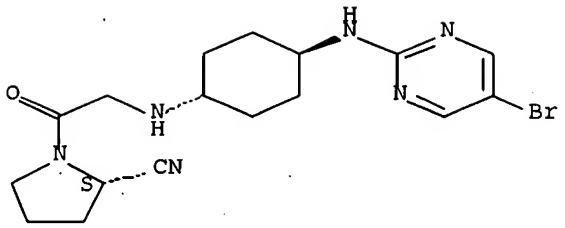


●2 HCl

RN 412284-90-3 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-bromo-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

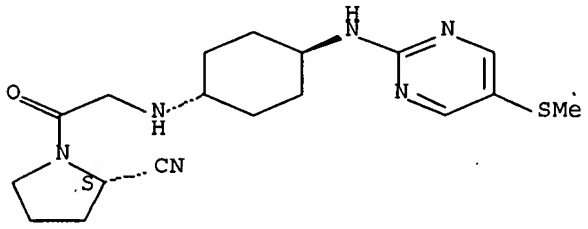
Absolute stereochemistry.



●2 HCl

RN 412284-91-4 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[5-(methylthio)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

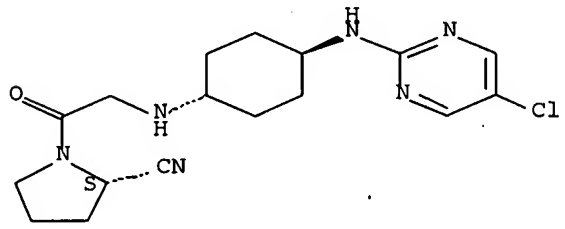
Absolute stereochemistry.



●2 HCl

RN 412284-92-5 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-chloro-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

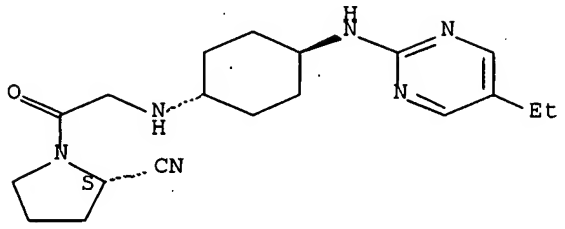
Absolute stereochemistry.



●2 HCl

RN 412285-02-0 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-ethyl-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

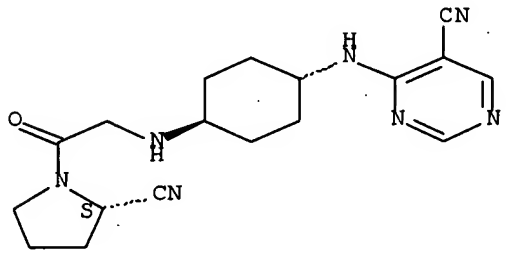
Absolute stereochemistry.



●2 HCl

RN 412285-03-1 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-cyano-4-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

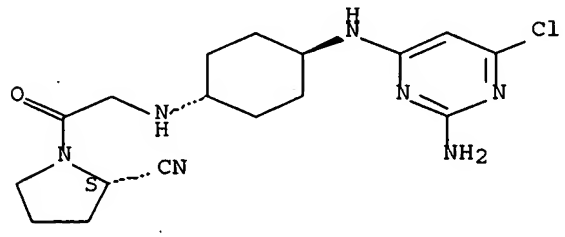
Absolute stereochemistry.



●2 HCl

RN 412285-05-3 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(2-amino-6-chloro-4-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

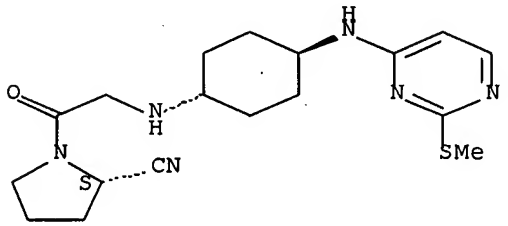


●2 HCl

RN 412285-08-6 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[2-(methylthio)-4-

pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

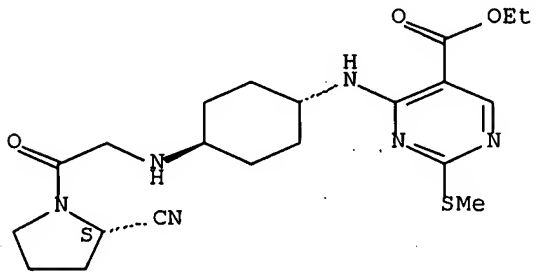
Absolute stereochemistry.



●2 HCl

RN 412285-09-7 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(methylthio)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

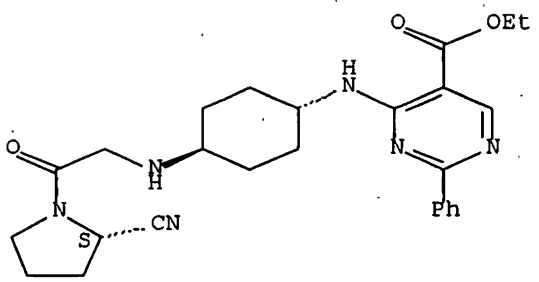
Absolute stereochemistry.



●2 HCl

RN 412285-11-1 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-phenyl-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

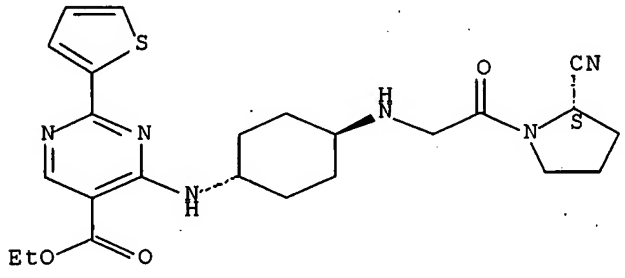
Absolute stereochemistry.



●2 HCl

RN 412285-12-2 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(2-thienyl)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

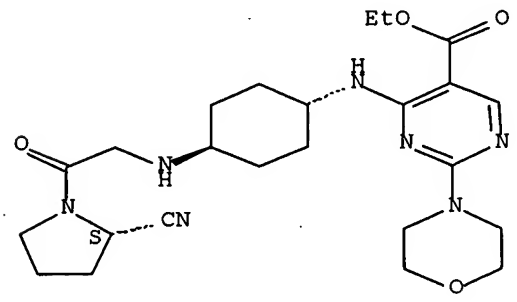
Absolute stereochemistry.



●2 HCl

RN 412285-13-3 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(4-morpholinyl)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

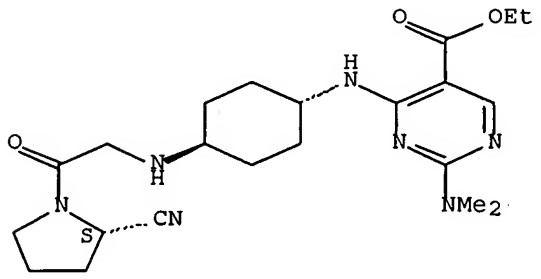
Absolute stereochemistry.



●2 HCl

RN 412285-14-4 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(dimethylamino)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

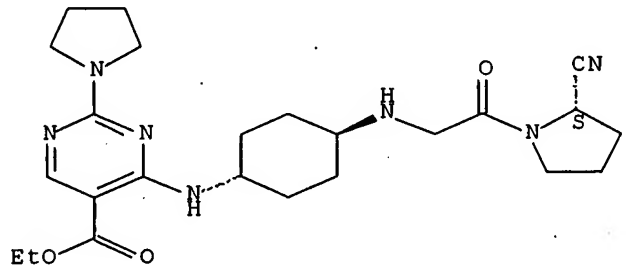
Absolute stereochemistry.



●2 HCl

RN 412285-15-5 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(1-pyrrolidinyl)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

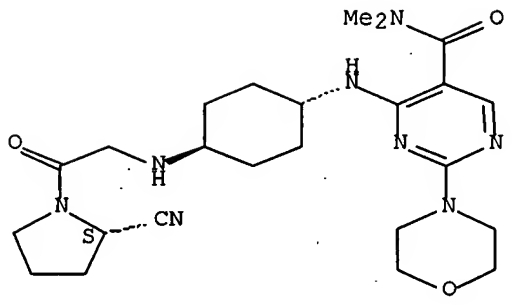
Absolute stereochemistry.



●2 HCl

RN 412285-16-6 CAPLUS
CN 5-Pyrimidinecarboxamide, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-N,N-dimethyl-2-(4-morpholinyl)-, dihydrochloride (9CI) (CA INDEX NAME)

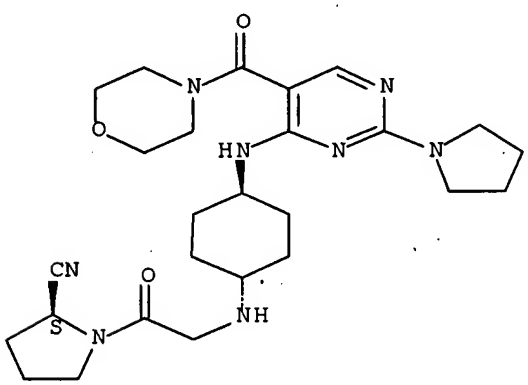
Absolute stereochemistry.



●2 HCl

RN 412285-17-7 CAPLUS
CN Morpholine, 4-[[4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(1-pyrrolidinyl)-5-pyrimidinyl]carbonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

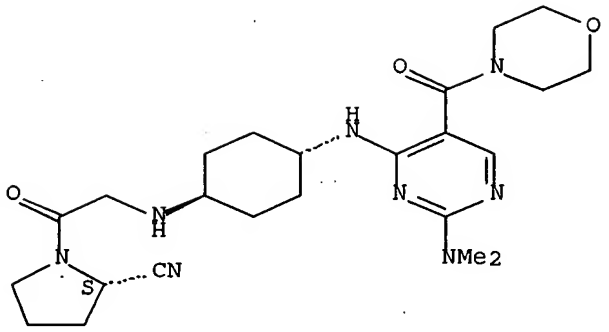
Absolute stereochemistry.



●2 HCl

RN 412285-18-8 CAPLUS
CN Morpholine, 4-[[4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(dimethylamino)-5-pyrimidinyl]carbonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

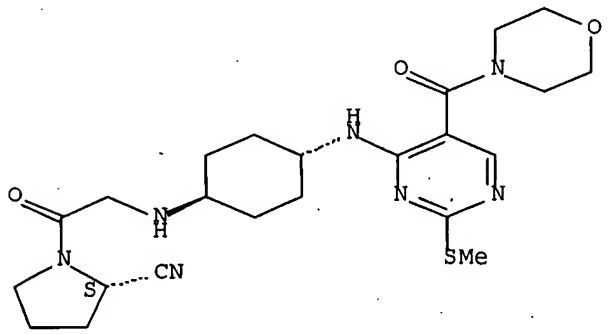
Absolute stereochemistry.



●2 HCl

RN 412285-19-9 CAPLUS
CN Morpholine, 4-[[4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(methylthio)-5-pyrimidinyl]carbonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

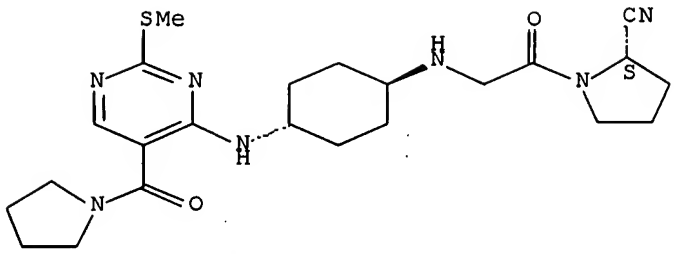
Absolute stereochemistry.



●2 HCl

RN 412285-20-2 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[2-(methylthio)-5-(1-pyrrolidinylcarbonyl)-4-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

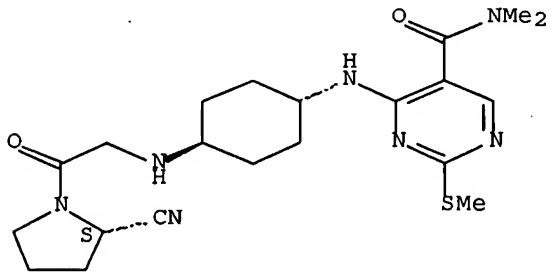
Absolute stereochemistry.



●2 HCl

RN 412285-21-3 CAPLUS
CN 5-Pyrimidinecarboxamide, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-N,N-dimethyl-2-(methylthio)-, dihydrochloride (9CI) (CA INDEX NAME)

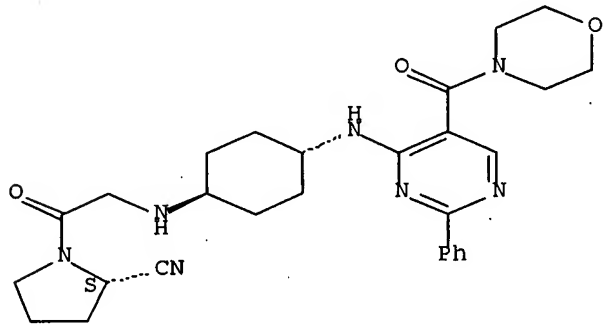
Absolute stereochemistry.



●2 HCl

RN 412285-22-4 CAPLUS
CN Morpholine, 4-[[4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-phenyl-5-pyrimidinyl]carbonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

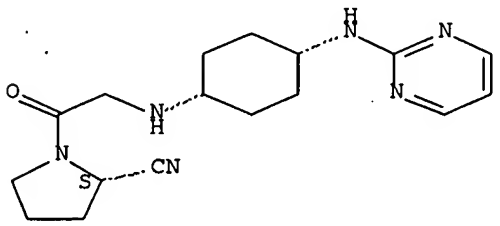
Absolute stereochemistry.



●2 HCl

RN 412285-43-9 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[cis-4-(2-pyrimidinylamino)cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

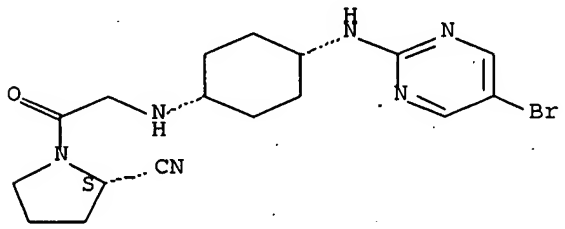
Absolute stereochemistry.



●2 HCl

RN 412285-44-0 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[cis-4-[(5-bromo-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

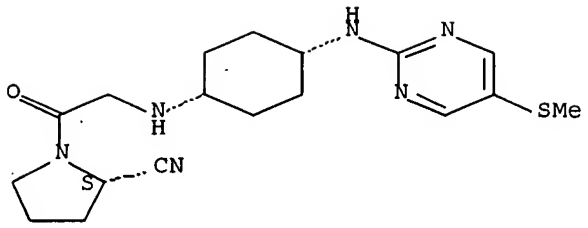
Absolute stereochemistry.



●2 HCl

RN 412285-45-1 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[cis-4-[[5-(methylthio)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

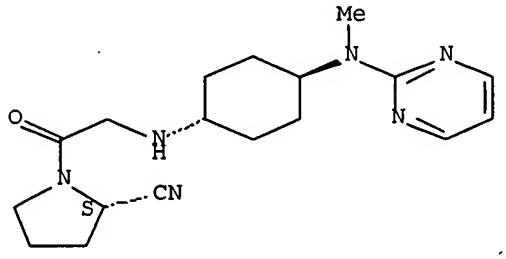
Absolute stereochemistry.



●2 HCl

RN 412285-64-4 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-(methyl-2-pyrimidinylamino)cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

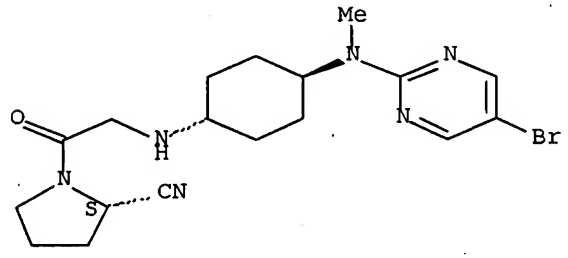
Absolute stereochemistry.



●2 HCl

RN 412285-65-5 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-bromo-2-pyrimidinyl)methylamino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

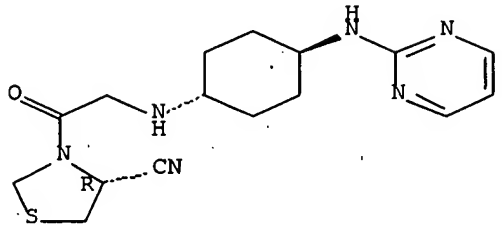
Absolute stereochemistry.



●2 HCl

RN 412288-75-6 CAPLUS
CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-(2-pyrimidinylamino)cyclohexyl]amino]acetyl]-, monohydrochloride, (4R)- (9CI) (CA INDEX NAME)

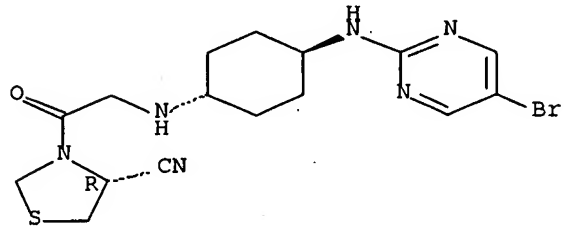
Absolute stereochemistry.



● HCl

RN 412288-76-7 CAPLUS
CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[(5-bromo-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

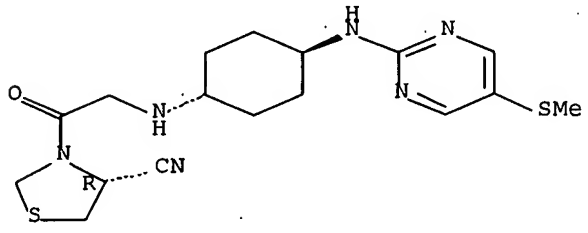
Absolute stereochemistry.



●2 HCl

RN 412288-77-8 CAPLUS
CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[[5-(methylthio)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

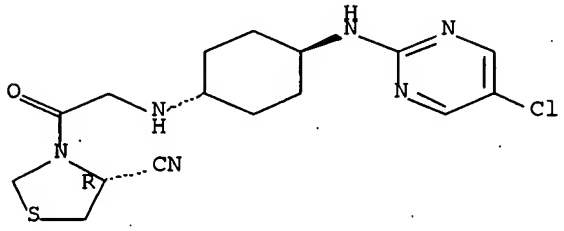


●2 HCl

RN 412288-78-9 CAPLUS
CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[(5-chloro-2-

pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

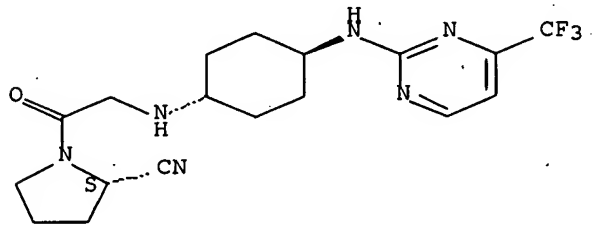
Absolute stereochemistry.



●2 HCl

RN 412915-48-1 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[4-(trifluoromethyl)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

L23 ANSWER 6 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:971736 CAPLUS Full-text
DOCUMENT NUMBER: 140:16656
TITLE: cis-N-(Quinolin-4-yl)cyclohexane-1,4-diamine derivatives as antagonists of melanin concentrating hormone (MCH) and their pharmaceutical compositions and therapeutic uses, e.g., for treatment of obesity
INVENTOR(S): Kym, Philip R.; Hartandi, Kresna; Gao, Ju; Phelan, Kathleen M.; Akritopoulou-Zanze, Irini; Collins, Christine A.; Vasudevan, Anil; Verzal, Mary K.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: U.S. Pat. Appl. Publ., 89 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 2003229119 A1 20031211 US 2003-372359 20030221 <--
US 6818772 B2 20041116
PRIORITY APPLN. INFO.: US 2002-359081P P 20020222 <--
OTHER SOURCE(S): MARPAT 140:16656
ED Entered STN: 14 Dec 2003
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

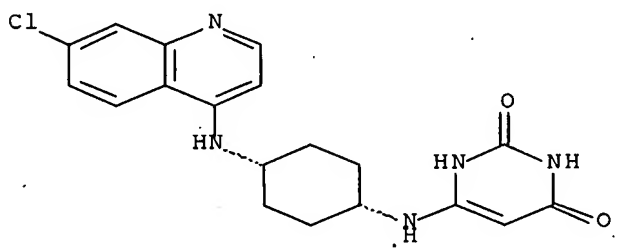
AB The invention is directed to the compds. of formula I, or therapeutically suitable salts, esters, prodrugs, or zwitterions thereof [R1, R2, R3 = H, alkyl, alkoxy, halo, haloalkyl, haloalkoxy, OH, NH2 and derivs.; R4 = H, alkyl; R5 = -(CH2)mYAB; m = 0-6; A = bond, alkoxyalkylene, alkylene, or hydroxyalkylene; B = H, alkyl, aryl, aroyl, arylsulfonyl, aralkenyl, aryloxyalkyl, biaryl, biarylalkyl, cycloalkyl, heterocyclyl, heterocyclylcarbonyl, heterocyclylsulfonyl, haloalkyl, NH2 or derivs., carbamoyl or derivs., OH or derivs., SH or derivs.; Y = CO, S, SO, SO2, or bond; R6 = H, alkyl, arylcarboxyalkyl; R7, R8, R9, R10 = H, alkyl, alkoxy, halo, haloalkyl, haloalkoxy, OH; or R7R8 = oxo; with 4 provisos]. The invention further relates to the antagonism of the effects of melanin-concentrating hormone (MCH) through the MCH receptor, which is useful for the prevention or treatment of eating disorders, weight gain, obesity, abnormalities in reproduction and sexual behavior, thyroid hormone secretion, diuresis and water/electrolyte homeostasis, sensory processing, memory, sleeping, arousal, anxiety, depression, seizures, neurodegeneration and psychiatric disorders. Approx. 450 synthetic examples of I are given. For instance, reaction of N-(7-chloroquinolin-4-yl)cyclohexane-1,4-diamine (cis isomer) with 4-chloro-2,8-bis(trifluoromethyl)quinoline in N-methylpyrrolidinone the presence of Et3N at 150° gave title compound II. In a fluorescence assay for release of intracellular Ca++ induced by activation of MCHR, a more preferred group of compds. I inhibited MCH-induced fluorescence in a range of 90-100% at 10 μM. A more preferred group of I also gave 90-100% inhibition of 125I-MCH binding to human MCHR1 at 2 μM (no addnl. data).

IT 589492-45-5P, cis-6-[[4-[(7-Chloroquinolin-4-yl)amino]cyclohexyl]amino]pyrimidine-2,4(1H,3H)-dione
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of quinolinylcyclohexanediamine derivs. as MCH receptor antagonists)

RN 589492-45-5 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 6-[[cis-4-[(7-chloro-4-quinolinyl)amino]cyclohexyl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

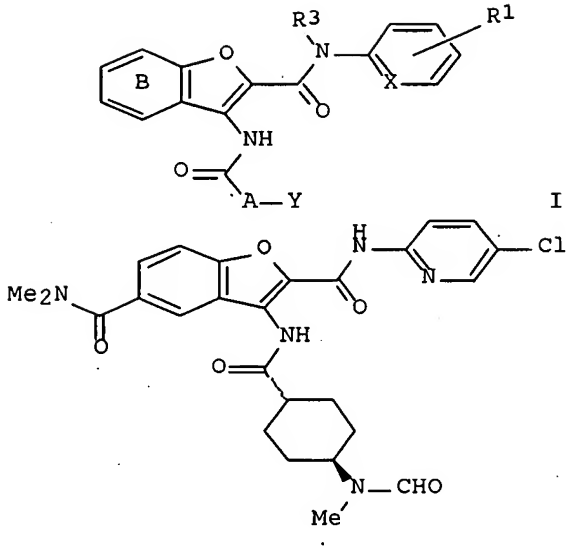


REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 7 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:796684 CAPLUS Full-text
DOCUMENT NUMBER: 139:292142
TITLE: Preparation of benzofuran derivatives as activated blood coagulation factor X inhibitors for treatment of thrombosis
INVENTOR(S): Kawaguchi, Takayuki; Akatsuka, Hidenori; Iijima, Toru; Tsuboi, Yasunori; Mitsui, Takashi; Murakami, Jun
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: PCT Int. Appl., 274 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003082847	A1	20031009	WO 2003-JP3807		20030327 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
JP 2004250417	A	20040909	JP 2003-84865		20030326 <--
CA 2479831	A1	20031009	CA 2003-2479831		20030327 <--
AU 2003221178	A1	20031013	AU 2003-221178		20030327 <--
EP 1489078	A1	20041222	EP 2003-712982		20030327 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
BR 2003008796	A	20050111	BR 2003-8796		20030327 <--
CN 1656086	A	20050817	CN 2003-811791		20030327 <--
NZ 535267	A	20060331	NZ 2003-535267		20030327 <--
RU 2286344	C2	20061027	RU 2004-131680		20030327 <--
ZA 2004007359	A	20050628	ZA 2004-7359		20040914 <--
US 2005282808	A1	20051222	US 2004-508512		20040921 <--
IN 2004CN02112	A	20060303	IN 2004-CN2112		20040922 <--
NO 2004004644	A	20041216	NO 2004-4644		20041027 <--
PRIORITY APPLN. INFO.:			JP 2002-91686	A	20020328 <--
			JP 2002-376158	A	20021226 <--
			WO 2003-JP3807	W	20030327

OTHER SOURCE(S): MARPAT 139:292142
ED Entered STN: 10 Oct 2003
GI



I

II

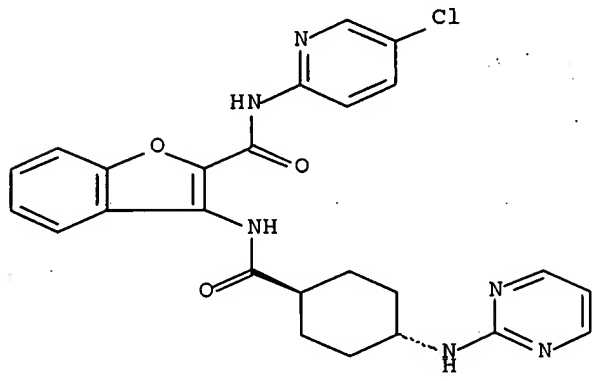
AB The title compds. I [wherein X = N or CH; Y = (un)substituted amino, cycloalkyl, or saturated heterocyclyl; A = a single bond, O, or hydrocarbyl; R1 = H, halo, alkyl, alkoxy, CN, or (un)substituted amino; ring B = (un)substituted Ph; R3 = H or alkyl] and pharmaceutically acceptable salts thereof are prepared as activated blood coagulation factor X (FXa) inhibitors. For example, the compound II was prepared in a multi-step synthesis. II showed IC50 of <100 nM against FXa. I are useful for the treatment of thrombosis (no data).

IT 609803-50-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of benzofuran derivs. as activated blood coagulation factor X inhibitors for treatment of thrombosis)

RN 609803-50-1 CAPLUS

CN 2-Benzofurancarboxamide, N-(5-chloro-2-pyridinyl)-3-[[[trans-4-(2-pyrimidinylamino)cyclohexyl]carbonyl]amino]-, dihydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



●2 HCl

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 8 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:678662 CAPLUS Full-text
DOCUMENT NUMBER: 139:214342
TITLE: cis-N-(Quinolin-4-yl)cyclohexane-1,4-diamine derivatives as antagonists of melanin concentrating hormone (MCH) and their pharmaceutical compositions and therapeutic uses, e.g., for treatment of obesity
INVENTOR(S): Kym, Philip R.; Hartandi, Kresna; Gao, Ju; Phelan, Kathleen M.; Akritopoulou-Zanze, Irini; Collins, Christine A.; Vasudevan, Anil; Verzal, Mary K.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 207 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003070244	A1	20030828	WO 2003-US5510	20030221 <--
W: CA, JP, MX				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR				
PRIORITY APPLN. INFO.:			US 2002-81675 A	20020222 <--

OTHER SOURCE(S): MARPAT 139:214342
ED Entered STN: 29 Aug 2003
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention is directed to the compds. of formula I, or therapeutically suitable salts, esters, prodrugs, or zwitterions thereof [R1, R2, R3 = H, alkyl, alkoxy, halo, haloalkyl, haloalkoxy, OH, NH2 and derivs.; R4 = H, alkyl; R5 = -(CH2)mYAB; m = 0-6; A = bond, alkoxyalkylene, alkylene, or hydroxyalkylene; B = H, alkyl, aryl, aroyl, arylsulfonyl, aralkenyl, aryloxyalkyl, biaryl, biarylalkyl, cycloalkyl, heterocyclyl, heterocyclylcarbonyl, heterocyclylsulfonyl, haloalkyl, NH2 or derivs., carbamoyl or derivs., OH or derivs., SH or derivs.; Y = CO, S, SO, SO2, or bond; R6 = H, alkyl, arylcarboxyalkyl; R7, R8, R9, R10 = H, alkyl, alkoxy, halo, haloalkyl, haloalkoxy, OH; or R7R8 = oxo; with 4 provisos]. The invention further relates to the antagonism of the effects of melanin-concentrating hormone (MCH) through the MCH receptor, which is useful for the prevention or treatment of eating disorders, weight gain, obesity, abnormalities in reproduction and sexual behavior, thyroid hormone secretion, diuresis and water/electrolyte homeostasis, sensory processing, memory, sleeping, arousal, anxiety, depression, seizures, neurodegeneration and psychiatric disorders. Approx. 450 synthetic examples of I are given. For instance, reaction of N-(7-chloroquinolin-4-yl)cyclohexane-1,4-diamine (cis isomer) with 4-chloro-2,8-bis(trifluoromethyl)quinoline in N-methylpyrrolidinone the presence of Et3N at 150° gave title compound II. In a fluorescence assay for release of intracellular Ca++ induced by activation of

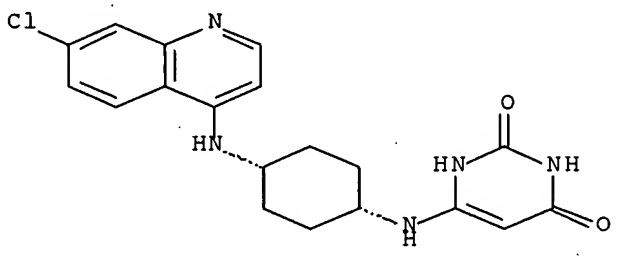
MCHR, a more preferred group of compds. I inhibited MCH-induced fluorescence in a range of 90-100% at 10 μM. A more preferred group of I also gave 90-100% inhibition of 125I-MCH binding to human MCHR1 at 2 μM (no addnl. data).

IT 589492-45-5P, cis-6-[[4-[(7-Chloroquinolin-4-yl)amino]cyclohexyl]amino]pyrimidine-2,4(1H,3H)-dione
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of quinolinylcyclohexanediamine derivs. as MCH receptor antagonists)

RN 589492-45-5 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, 6-[[cis-4-[(7-chloro-4-quinolinyl)amino]cyclohexyl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 9 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:610204 CAPLUS Full-text

DOCUMENT NUMBER: 139:164801

TITLE: Preparation of 2,4-pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of allergic diseases, inflammatory conditions, and tissue destruction

INVENTOR(S): Singh, Rajinder; Argade, Ankush; Payan, Donald G.; Molineaux, Susan; Holland, Sacha J.; Clough, Jeffrey; Keim, Holger; Bhamidipati, Somasekhar; Sylvain, Catherine; Li, Weigun; Rossi, Alexander B.

PATENT ASSIGNEE(S): Rigel Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 648 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003063794	A2	20030807	WO 2003-US3022	20030131 <--
WO 2003063794	A3	20031204		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2474277	A1	20030807	CA 2003-2474277		20030131 <--
US 2004029902	A1	20040212	US 2003-355543		20030131 <--
EP 1471915	A2	20041103	EP 2003-707654		20030131 <--
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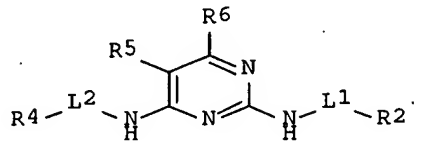
JP 2005516046	T	20050602	JP 2003-563490		20030131 <--
CN 1625400	A	20050608	CN 2003-803180		20030131 <--
BR 2003007355	A	20060411	BR 2003-7355		20030131 <--
US 2005038243	A1	20050217	US 2004-858343		20040601 <--
US 7060827	B2	20060613			
US 2005209230	A1	20050922	US 2004-911684		20040803 <--
IN 2004KN01139	A	20060512	IN 2004-KN1139		20040809 <--
NO 2004003632	A	20041026	NO 2004-3632		20040831 <--
US 2006025410	A1	20060202	US 2005-149105		20050608 <--
US 2006035916	A1	20060216	US 2005-148746		20050608 <--
US 2006058292	A1	20060316	US 2005-149418		20050608 <--
US 2006135543	A1	20060622	US 2005-299207		20051208 <--
PRIORITY APPLN. INFO.:			US 2002-353267P	P	20020201 <--
			US 2002-353333P	P	20020201 <--
			US 2002-399673P	P	20020729 <--
			US 2002-434277P	P	20021217 <--
			US 2003-355543	A1	20030131
			WO 2003-US3022	W	20030131
			US 2004-858343	A3	20040601

OTHER SOURCE(S): MARPAT 139:164801
ED Entered STN: 08 Aug 2003
GI



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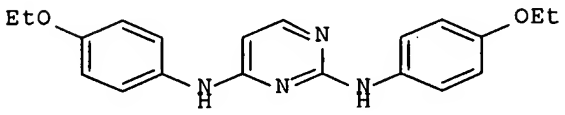


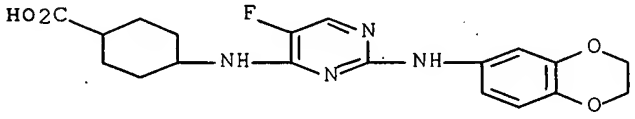
II

AB Title compds. I [wherein L1 and L2 = independently a bond or a linker; R2 = (un)substituted alkyl, (hetero)cycloalkyl, or (hetero)aryl; R4 = H or R2; R5 = R6 or (un)substituted alkyl, alkenyl, or alkynyl; R6 = independently H, an electroneg. group, protected alc. or thiol, haloalkyl(oxy), halo, CN, NC, OCN, SCN, NO, NO2, N3, or (un)substituted amino, sulfamoyl(oxy), acyl, carboxy, carbamoyl, (hetero)aryl(alkyl), etc.; with provisos and exclusions; and salts, hydrates, solvates, N-oxides, and prodrugs thereof] were prepared as inhibitors of the IgE and/or IgG receptor signaling cascades that lead to the release of chemical mediators. For example, coupling of 2,4-dichloropyrimidine with 4-ethoxyaniline in EtOH provided N2,N4-bis(4-

ethoxyphenyl)-2,4- pyrimidinediamine (II). The latter inhibited degranulation of bone marrow derived mast cells challenged with anti-IgE and ionomycin with IC50 values of 4.5 μM and 4.4 μM, resp. Thus, I and their pharmaceutical compns. are useful in the treatment and prevention of diseases characterized by, caused by, or associated with the release of chemical mediators via degranulation of mast, basophil, neutrophil, or eosinophil cells and other processes effected by activation of the IgE and/or IgG receptor signaling cascades. The treatment and prevention of allergic diseases, low grade scarring, diseases associated with tissue destruction, diseases associated with tissue inflammation, inflammation, and scarring are targeted uses (no data).

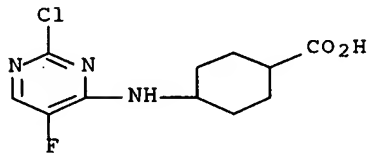
IT 575476-86-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(IgE and/or IgG receptor modulator; preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of allergic diseases, inflammatory conditions, and tissue destruction)

RN 575476-86-7 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[2-[(2,3-dihydro-1,4-benzodioxin-6-yl)amino]-5-fluoro-4-pyrimidinyl]amino]- (CA INDEX NAME)



IT 575476-87-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidinediamines as IgE and/or IgG receptor modulators for treatment of allergic diseases, inflammatory conditions, and tissue destruction)

RN 575476-87-8 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[(2-chloro-5-fluoro-4-pyrimidinyl)amino]- (9CI) (CA INDEX NAME)

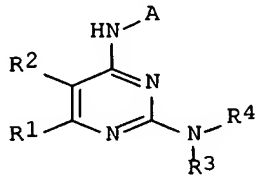


L23 ANSWER 10 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:532524 CAPLUS Full-text
DOCUMENT NUMBER: 139:101141
TITLE: Preparation of 2,4-diaminopyrimidines as inhibitors of prolylpeptidase, inducers of apoptosis and cancer treatment agents
INVENTOR(S): Dumas, Jacques; Dixon, Julie; Sibley, Robert; Wood, Jill

PATENT ASSIGNEE(S): Bayer Corporation, USA
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003055489	A1	20030710	WO 2002-US41146	20021220 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002367172	A1	20030715	AU 2002-367172	20021220 <--
PRIORITY APPLN. INFO.:			US 2001-343047P P	20011221 <--
			WO 2002-US41146 W	20021220 <--

OTHER SOURCE(S): MARPAT 139:101141
ED Entered STN: 11 Jul 2003
GI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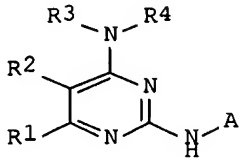
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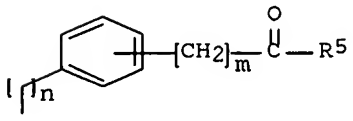
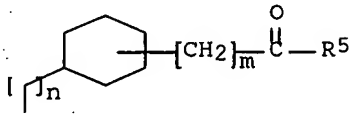

III


IV

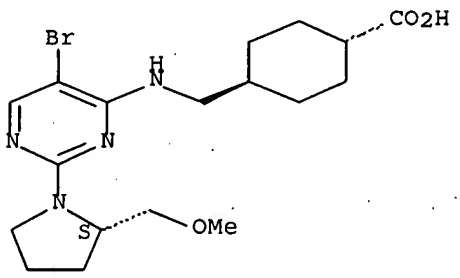
AB The title compds. [I or II; R1, R2 = H, halo, OH, etc.; R3 = H; R4 = (un)substituted alkyl, cycloalkyl, aryl, alkylaryl; or NR3R4 = (un)saturated 4-8 membered heterocyclyl which optionally contains 1-3 addnl. heteroatoms selected from N, O and S; A = III or IV; R5 = OH, OR6, NR8R9; R6 = alkyl, haloalkyl, aryl, haloaryl; R8, R9 = H, alkyl, aryl, etc.; n, m = 0-1], useful for the inhibiting prolylpeptidase, inducing apoptosis and treating cancer, were prepared E.g., a 3-step synthesis of I [A = 4-(HO2C)C6H4CH2; R1 = H; R2 = Me; R3 = H; R4 = 2-thienylmethyl], starting from Me 4-(aminomethyl)benzoate and 2,4-dichloro-5-methylpyrimidine, was given. All exemplified compds. I were found to inhibit prolylpeptidase at or below of 10 μM.

IT 557789-86-3P 557789-87-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2,4-diaminopyrimidines as inhibitors of prolylpeptidase, inducers of apoptosis and cancer treatment agents)

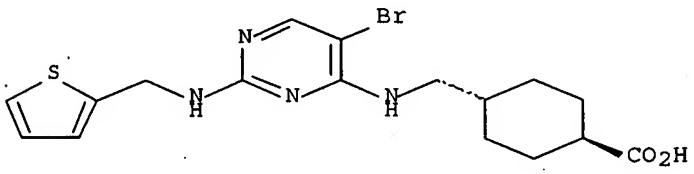
RN 557789-86-3 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[[5-bromo-2-[(2S)-2-(methoxymethyl)-1-pyrrolidinyl]-4-pyrimidinyl]amino]methyl]-, trans- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 557789-87-4 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[[5-bromo-2-[(2-thienylmethyl)amino]-4-pyrimidinyl]amino]methyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 11 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:511301 CAPLUS Full-text
DOCUMENT NUMBER: 139:85041
TITLE: Heteroaryl-substituted aminocyclohexane derivatives as inhibitors of 2,3-oxidosqualene lanosterol cyclase
INVENTOR(S): Ackermann, Jean; Aebi, Johannes; Dehmlow, Henrietta; Maerki, Hans-Peter; Morand, Olivier
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: PCT Int. Appl., 83 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003053933	A1	20030703	WO 2002-EP14037	20021211 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
UG, UZ, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ,
CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US 2003186984	A1	20031002	US 2002-310559		20021205 <--
US 7012077	B2	20060314			
CA 2469380	A1	20030703	CA 2002-2469380		20021211 <--
AU 2002366732	A1	20030709	AU 2002-366732		20021211 <--
EP 1458683	A1	20040922	EP 2002-790481		20021211 <--
EP 1458683	B1	20061122			
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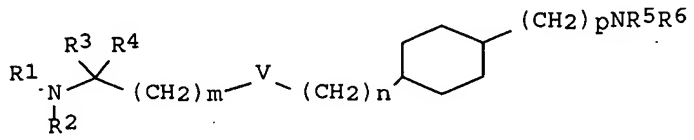
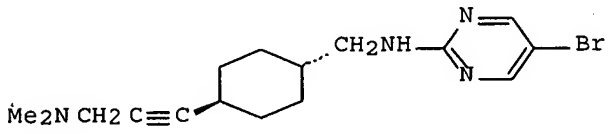
BR 2002015257	A	20041207	BR 2002-15257		20021211 <--
CN 1610669	A	20050427	CN 2002-825665		20021211 <--
JP 2005517667	T	20050616	JP 2003-554649		20021211 <--
RU 2286987	C2	20061110	RU 2004-122480		20021211 <--
AT 346045	T	20061215	AT 2002-790481		20021211 <--
PRIORITY APPLN. INFO.:			EP 2001-130284	A	20011220 <--
			WO 2002-EP14037	W	20021211 <--

OTHER SOURCE(S): MARPAT 139:85041
ED Entered STN: 04 Jul 2003
GI



I



II

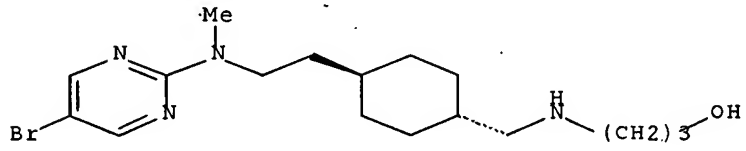
AB Title compds. I [R1 = H, alkyl, hydroxyalkyl, alkenyl; R2 = (un)substituted alkyl, cycloalkyl, cycloalkylalkyl, alkenyl; NR1R2 = heterocyclic; R3, R4 = H, alkyl; R3R4 = (CH2)5; R5 = H, alkyl, alkenyl; R6 = (un)substituted pyridinyl, pyridazinyl, pyrimidinyl, pyrazinyl; V = bond, O, S, CH:CHCH2O, CH:CH, C.tplbond.C; m, n = 0-7; p = 0-2] and their N-oxides were prepared for use as 2,3-oxidosqualene lanosterol cyclase inhibitors in treating diseases such as hypercholesterolemia, hyperlipemia, arteriosclerosis, vascular diseases, mycoses, parasitic infections, gallstones, tumors and/or hyperproliferative disorders, and treatment and/or prophylaxis of impaired glucose tolerance and diabetes. Thus, trans-3-{4-[(5-bromo-2-pyrimidinyl)methylamino]cyclohexyl}prop-2-yn- 1-ol, prepared from trans-4-tert.-butoxycarbonylaminocyclohexanecarboxylic acid and 2,5-dibromopyrimidine via trans-3-(4-methylaminocyclohexyl)prop-2- yn-1-ol, was converted to its mesylate and treated with Me2NH to give the title compound II.

IT 553677-39-7P 553677-40-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation of heteroaryl-substituted aminocyclohexane derivs. as inhibitors of 2,3-oxidosqualene lanosterol cyclase)

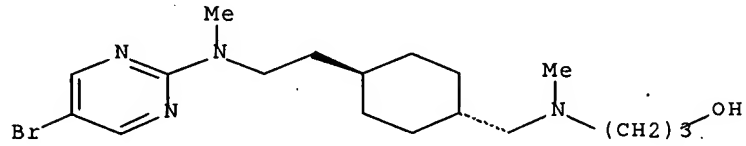
RN 553677-39-7 CAPLUS
CN 1-Propanol, 3-[[[trans-4-[2-[(5-bromo-2-pyrimidinyl)methylamino]ethyl]cyclohexyl]methyl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 553677-40-0 CAPLUS
CN 1-Propanol, 3-[[[trans-4-[2-[(5-bromo-2-pyrimidinyl)methylamino]ethyl]cyclohexyl]methyl]methylamino]- (9CI) (CA INDEX NAME)

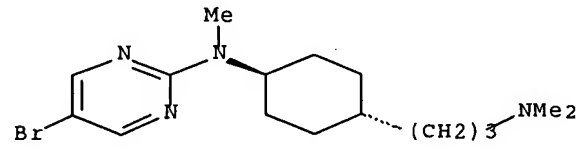
Relative stereochemistry.



IT 553676-54-3P 553676-55-4P 553676-56-5P
553676-57-6P 553676-71-4P 553677-00-2P
553677-02-4P 553677-37-5P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heteroaryl-substituted aminocyclohexane derivs. as inhibitors of 2,3-oxidosqualene lanosterol cyclase)

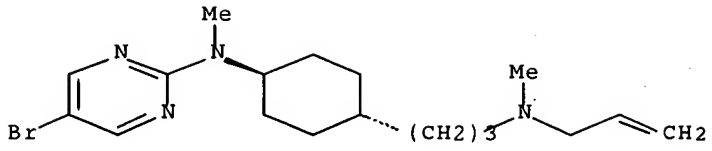
RN 553676-54-3 CAPLUS
CN 2-Pyrimidinamine, 5-bromo-N-[trans-4-[3-(dimethylamino)propyl]cyclohexyl]-N-methyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



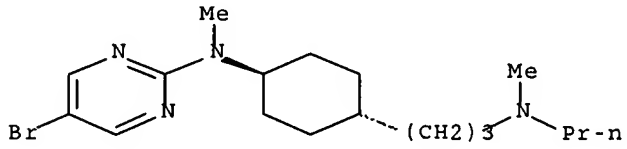
RN 553676-55-4 CAPLUS
CN 2-Pyrimidinamine, 5-bromo-N-methyl-N-[trans-4-[3-(methyl-2-propenylamino)propyl]cyclohexyl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



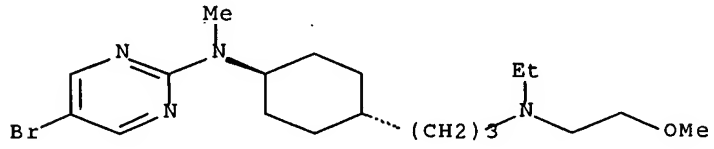
RN 553676-56-5 CAPLUS
CN 2-Pyrimidinamine, 5-bromo-N-methyl-N-[trans-4-[3-(methylpropylamino)propyl]cyclohexyl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



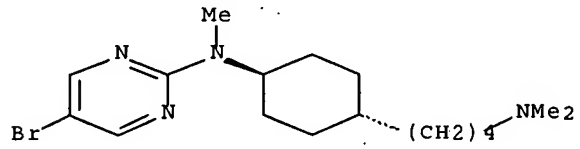
RN 553676-57-6 CAPLUS
CN 2-Pyrimidinamine, 5-bromo-N-[trans-4-[3-[ethyl(2-methoxyethyl)amino]propyl]cyclohexyl]-N-methyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



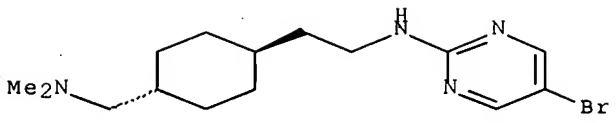
RN 553676-71-4 CAPLUS
CN 2-Pyrimidinamine, 5-bromo-N-[trans-4-[4-(dimethylamino)butyl]cyclohexyl]-N-methyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



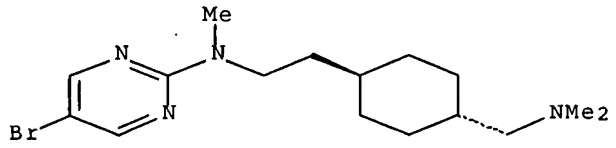
RN 553677-00-2 CAPLUS
CN 2-Pyrimidinamine, 5-bromo-N-[2-[trans-4-[(dimethylamino)methyl]cyclohexyl]ethyl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



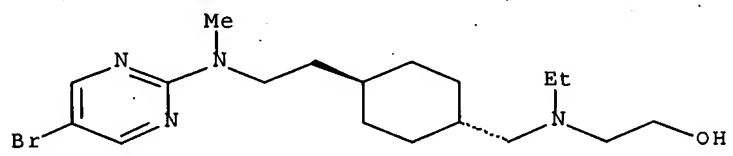
RN 553677-02-4 CAPLUS
CN 2-Pyrimidinamine, 5-bromo-N-[2-[trans-4-[(dimethylamino)methyl]cyclohexyl]ethyl]-N-methyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 553677-37-5 CAPLUS
CN Ethanol, 2-[[[trans-4-[2-[(5-bromo-2-pyrimidinyl)methylamino]ethyl]cyclohexyl]methyl]ethylamino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 12 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:376852 CAPLUS Full-text
DOCUMENT NUMBER: 138:385443
TITLE: Preparation of amino imidazolyl pyrimidinecarboxaldehyde thiosemicarbazones, pyridine analogs and related compounds as inhibitors of IkB kinases
INVENTOR(S): Hawley, Ronald Charles; Labadie, Sharada Shenvi; Sjogren, Eric Brian; Talamas, Francisco Xavier
PATENT ASSIGNEE(S): F. Hoffmann-La Roche AG, Switz.
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003040131	A1	20030515	WO 2002-EP12164	20021031 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				

CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

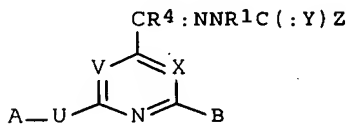
CA 2465711	A1	20030515	CA 2002-2465711	20021031 <--
AU 2002350657	A1	20030519	AU 2002-350657	20021031 <--
EP 1444223	A1	20040811	EP 2002-785344	20021031 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002013899	A	20040831	BR 2002-13899	20021031 <--
CN 1582284	A	20050216	CN 2002-822194	20021031 <--
JP 2005511608	T	20050428	JP 2003-542177	20021031 <--
US 2003144303	A1	20030731	US 2002-288968	20021106 <--
US 6846828	B2	20050125		
US 2005107403	A1	20050519	US 2004-967430	20041018 <--
US 7157580	B2	20070102		

PRIORITY APPLN. INFO.:	US 2001-338312P	P	20011107 <--
	WO 2002-EP12164	W	20021031 <--
	US 2002-288968	A3	20021106 <--

OTHER SOURCE(S): MARPAT 138:385443

ED Entered STN: 16 May 2003

GI



I

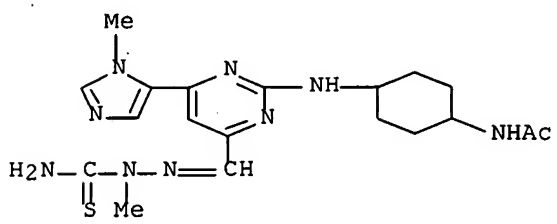
AB The present invention relates to aminopyrimidine and aminopyridine derivs. (shown as I; variables defined below; e.g. 2-butylamino-6-(1-methyl-1H-imidazol-5-yl)pyrimidine-4-carboxaldehyde 2-methylthiosemicarbazone (1)) and methods for their preparation The compds. are useful as inhibitors of IkB kinases and, therefore, may be used for the treatment of inflammatory, metabolic or malignant conditions (e.g. rheumatoid arthritis, inflammatory bowel disease, psoriasis, cancer, diabetes and septic shock). IC50 values for inhibition of IKKβ enzyme activity are reported for 3 examples of I; e.g. 0.314 μM for 1. Eleven example prepns. of intermediates and I and characterization data for .apprx.150 I are included. For example, 2-isopropylamino-6-(1-methyl-1H-imidazol-5-yl)pyrimidine-4-carboxaldehyde 2-methylthiosemicarbazone was prepared in 7 steps starting from Et diethoxyacetate, thiourea and benzyl bromide giving 2-benzylsulfanyl-6-diethoxymethylpyrimidin-4-ol as the 1st intermediate (50%); this intermediate was sequentially converted to the chloride (74%), pyrimidine imidazole, sulfone (31% for 2 steps), amino pyrimidine acetal (66%), aldehyde (64%) and finally the aldehyde thiosemicarbazone (71%). For I: one of either V or X is N and the other is CRa, or both V and X are CRa (Ra = H, (C1-C6)alkyl, (C3-C7)cycloalkyl or (C3-C7)cycloalkyl(C1-C6)alkyl); Y is O, S or NR (R is H, CN, NO2, (C1-C10)alkyl, (C3-C7)cycloalkyl, (C3-C7)cycloalkyl-(C1-C6)alkyl, (C3-C10)alkenyl or (C2-C10)alkynyl). Z is H, (C1-C6)alkyl, (C3-C7)cycloalkyl, (C3-C6)cycloalkyl(C1-C6)alkyl, (C2-C6)alkenyl, (C2-C6)alkynyl or N(R2)(R3); R1

is H, (C1-C10)alkyl, (C3-C10)alkenyl, (C2-C10)alkynyl, (C3-C7)cycloalkyl, (C3-C7)cycloalkyl(C1- C6)alkyl, (C1-C10)heteroalkyl, heterocyclyl, heterocyclyl (C1-C6)alkyl, aryl, aryl(C1-C4)alkyl, aryl(C1-C4) heteroalkyl, heteroaryl(C1-C4)alkyl, heteroaryl(C1-C4)heteroalkyl, C(O)R11 or (C1-C6)alkylene-C(O)R11;. R4 is H, (C1-C6)alkyl, (C3-C7)cycloalkyl, (C3-C7)cycloalkyl(C1-C6)alkyl, (C2-C6)alkenyl or (C2-C6)alkynyl; A is H, (C1-C10)alkyl, (C3-C10)alkenyl, (C2-C10)alkynyl, halo (C1-C6) alkyl, (C3-C7)cycloalkyl, (C3-C7)cycloalkyl(C1-C6)alkyl, (C1-C10)heteroalkyl, heterocyclyl, heterocyclyl(C1-C6) alkyl, heterosubstituted (C3-C7)cycloalkyl, aryl, aryl(C1-C4)alkyl, aryl(C1-C4)heteroalkyl, heteroaryl, heteroaryl(C1- C4)alkyl, heteroaryl(C1-C4)heteroalkyl or RaRbNC(:X) (Ra and Rb = H, (C1-C4)alkyl or aryl). X is O or S; B is a (un)substituted five- or six-membered aromatic ring containing at least 1 N and 0-3 addnl. heteroatoms, wherein the B ring substituents = halogen, CF3, CF3O, (C1-C6)alkyl, amino, (C1-C6)alkylamino, di(C1-C6)alkylamino, cyano, nitro, sulfonamido, acyl, acylamino and carboxamido; U is -NR5-, -O- or -S-; addnl. details are given in the claims.

IT 525559-73-3P, 2-((4-(Acetylamino)cyclohexyl)amino)-6-(1-methyl-1H-imidazol-5-yl)pyrimidine-4-carboxaldehyde 2-methylthiosemicarbazone 525559-79-9P, 2-((4-((Methylsulfonyl)amino)cyclohexyl)amino)-6-(1-methyl-1H-imidazol-5-yl)pyrimidine-4-carboxaldehyde 2-methylthiosemicarbazone 525560-05-8P, 2-((3-((Methylsulfonyl)amino)cyclohexyl)amino)-6-(1-methyl-1H-imidazol-5-yl)pyrimidine-4-carboxaldehyde 2-methylthiosemicarbazone
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of amino imidazolyl pyrimidinecarboxaldehyde thiosemicarbazones, pyridine analogs and related compds. as inhibitors of IkB kinases)

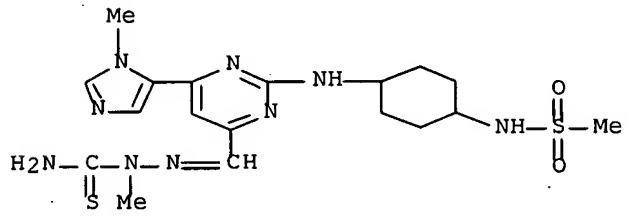
RN 525559-73-3 CAPLUS

CN Acetamide, N-[4-[[4-[[(aminothioxomethyl)methylhydrazono]methyl]-6-(1-methyl-1H-imidazol-5-yl)-2-pyrimidinyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

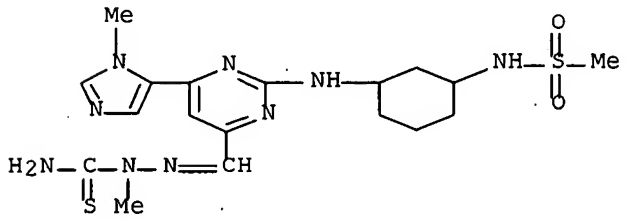


RN 525559-79-9 CAPLUS

CN Hydrazinecarbothioamide, 1-methyl-2-[[6-(1-methyl-1H-imidazol-5-yl)-2-[[4-[(methylsulfonyl)amino]cyclohexyl]amino]-4-pyrimidinyl]methylene]- (9CI) (CA INDEX NAME)



RN 525560-05-8 CAPLUS
CN Hydrazinecarbothioamide, 1-methyl-2-[[6-(1-methyl-1H-imidazol-5-yl)-2-[[3-[(methylsulfonyl)amino]cyclohexyl]amino]-4-pyrimidinyl]methylene]- (9CI) (CA INDEX NAME)



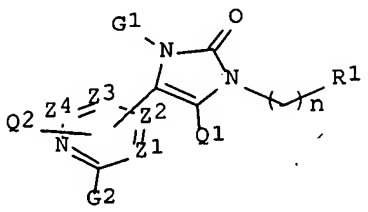
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 13 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:335096 CAPLUS Full-text
DOCUMENT NUMBER: 138:353990
TITLE: Preparation of 4-imidazolin-2-one derivatives as MAP kinase inhibitors
INVENTOR(S): Kubo, Akira; Imashiro, Ritsuo; Sakurai, Hiroaki; Miyoshi, Hidetaka; Ogasawara, Akihito; Hiramatsu, Hajime
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: PCT Int. Appl., 137 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003035638	A1	20030501	WO 2002-JP10937	20021022 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2461100	A1	20030501	CA 2002-2461100	20021022 <--
AU 2002363108	A1	20030506	AU 2002-363108	20021022 <--
EP 1439174	A1	20040721	EP 2002-802049	20021022 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002013465	A	20041109	BR 2002-13465	20021022 <--
CN 1571781	A	20050126	CN 2002-820837	20021022 <--
HU 200401949	A2	20050128	HU 2004-1949	20021022 <--
US 2004204426	A1	20041014	US 2004-827294	20040420 <--

NO 2004002010 A 20040709 NO 2004-2010 20040514 <--
PRIORITY APPLN. INFO.: JP 2001-324029 A 20011022 <--
JP 2002-263680 A 20020910 <--
WO 2002-JP10937 W 20021022 <--
JP 2003-116076 A 20030421

OTHER SOURCE(S): MARPAT 138:353990
ED Entered STN: 02 May 2003
GI



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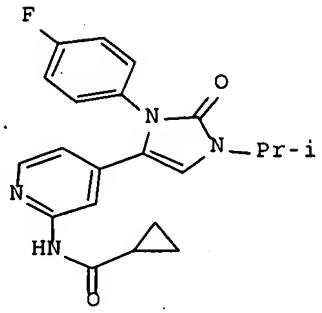


II

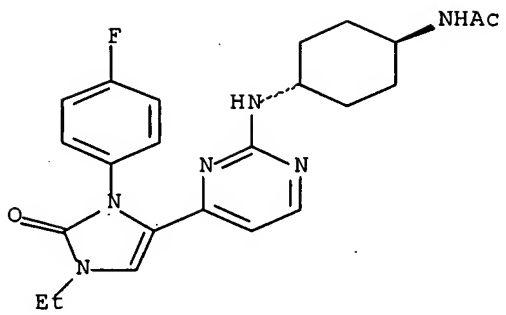
AB The title compds. I [wherein G1 = (un)substituted alkyl or B-W; B = (un)substituted Ph, Naphthyl, aromatic heterocyclyl, or cycloalkyl; W = a single bond or (un)substituted alkylene; Q1 and Q2 = independently H, halo, or alkyl; n = 0-4; R1 = H, (un)substituted (cyclo)alkyl, Ph, or heterocyclyl; Z1-Z4 = independently CH or N with exclusions; G2 = H, NR3R4, OR5, SR5, COR6, CHR7R8, or heterocyclyl; R3-R8 = independently H, alkenyl, alkynyl, OH, alkoxy, alkoxyoxalyl, alkylsulfonyl, (un)substituted alkyl, amino, alkanoyl, carbamoyl, cycloalkyl, Ph, heterocyclyl(carbonyl), PhCO, or heterocyclyl-CO] and pharmaceutically acceptable salts are prepared as mitogen activation proteins (MAP) kinase inhibitors. For example, the compound II•HCl was prepared in a multi-step synthesis. II•HCl showed 69% inhibitory activity against TNF-α in rat in the amount of 1 mg/kg after 90 min.

IT 521090-75-5P 521090-76-6P 521091-56-5P
521091-59-8P 521091-62-3P 521091-63-4P
521091-65-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(MAP kinase inhibitor; preparation of imidazolinone derivs. as MAP kinase inhibitors)

RN 521090-75-5 CAPLUS

CN Acetamide, N-[trans-4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

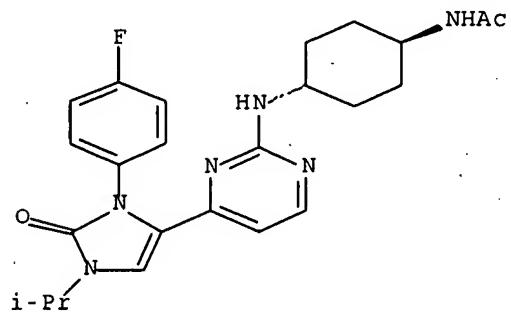
Relative stereochemistry.



● HCl

RN 521090-76-6 CAPLUS
CN Acetamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(1-methylethyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

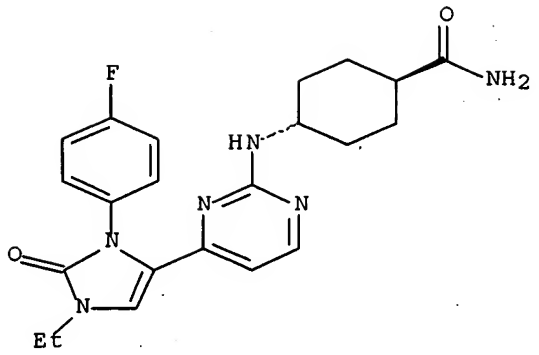
Relative stereochemistry.



● HCl

RN 521091-56-5 CAPLUS
CN Cyclohexanecarboxamide, 4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]-, monohydrochloride, trans- (9CI) (CA INDEX NAME)

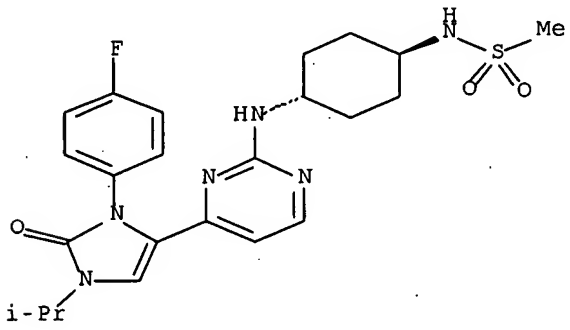
Relative stereochemistry.



● HCl

RN 521091-59-8 CAPLUS
CN Methanesulfonamide, N-[trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(1-methylethyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

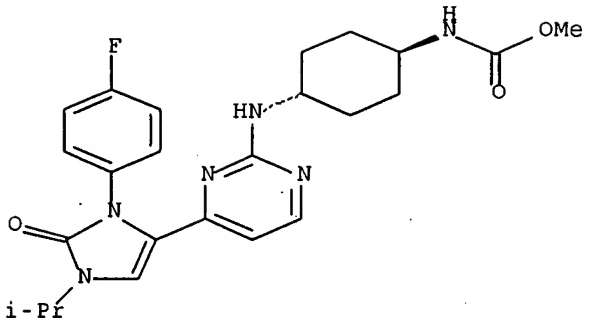
Relative stereochemistry.



● HCl

RN 521091-62-3 CAPLUS
CN Carbamic acid, [trans-4-[[4-[3-(4-fluorophenyl)-2,3-dihydro-1-(1-methylethyl)-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

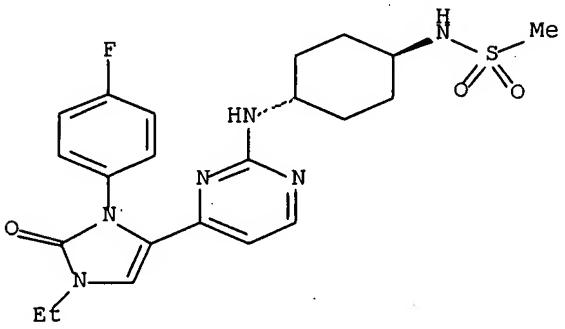
Relative stereochemistry.



● HCl

RN 521091-63-4 CAPLUS
CN Methanesulfonamide, N-[trans-4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, monohydrochloride (9CI) (CA INDEX NAME)

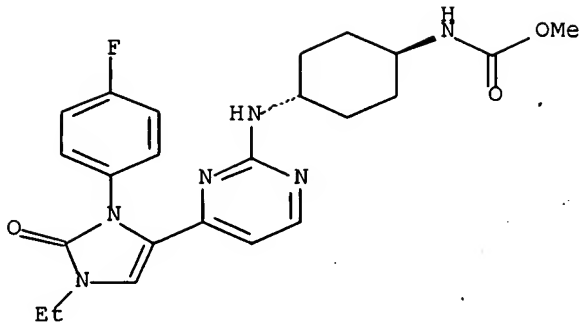
Relative stereochemistry.



● HCl

RN 521091-65-6 CAPLUS
CN Carbamic acid, [trans-4-[[4-[1-ethyl-3-(4-fluorophenyl)-2,3-dihydro-2-oxo-1H-imidazol-4-yl]-2-pyrimidinyl]amino]cyclohexyl]-, methyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

REFERENCE COUNT: 99 THERE ARE 99 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 14 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:319721 CAPLUS Full-text
DOCUMENT NUMBER: 138:321292
TITLE: Preparation of 2,4,5-trisubstituted pyrimidines as cyclin dependent kinase inhibitors
INVENTOR(S): Dahmann, Georg; Himmelsbach, Frank; Wittneben, Helmut; Pautsch, Alexander; Prokopowicz, Anthony S.; Krist, Bernd; Schnapp, Gisela; Steegmaier, Martin; Lenter, Martin; Schoop, Andreas; Steurer, Steffen; Spevak, Walter
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany; Boehringer Ingelheim Pharmaceuticals, Inc.; Boehringer Ingelheim International G.m.b.H.
SOURCE: PCT Int. Appl., 278 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003032997	A1	20030424	WO 2002-EP11453	20021014 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2463989	A1	20030424	CA 2002-2463989	20021014 <--
AU 2002340560	A1	20030428	AU 2002-340560	20021014 <--
EP 1438053	A1	20040721	EP 2002-774710	20021014 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2005509624	T	20050414	JP 2003-535800	20021014 <--
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US 7173028 B2 20070206
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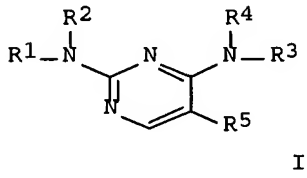
PRIORITY APPLN. INFO.: US 2001-330145P P 20011017 <--
WO 2002-EP11453 W 20021014 <--
US 2002-271763 A3 20021016 <--
OTHER SOURCE(S): MARPAT 138:321292
ED Entered STN: 25 Apr 2003
GI



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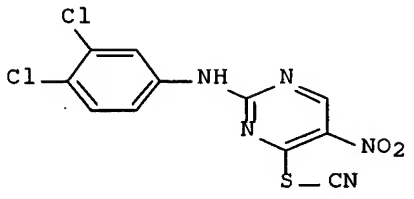

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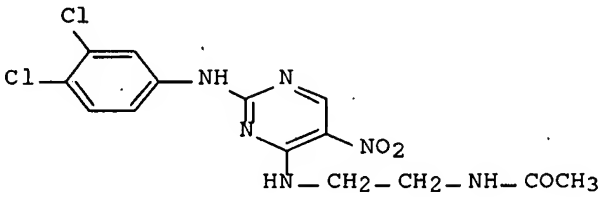


III

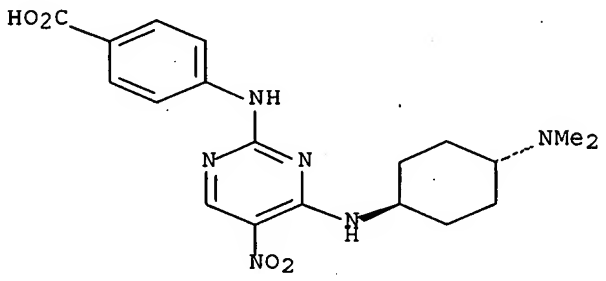
AB Title compds. I [R1 = H, alkyl; R2 = (un)substituted alkyl; R3 = H, alkyl; R4 = (un)substituted alkyl; R5 = halo] and their pharmaceutically acceptable salts were prepared For example, condensation of thiocyanatopyrimide II, e.g., prepared from 3,4-dichloroaniline and 2-chloro-4-thiocyanato-5-nitropyrimidine in one step, and acetylaminoethylamine provided trisubstituted pyrimidine III in 88% yield. In CDK1/CyclinB1 kinase inhibition studies, 88-examples of compds. I exhibited IC50 values more than 100 nM. Compds. I are claimed useful for the treatment of diseases characterized by abnormal cell proliferation.

IT 514830-77-4P, 2-(4-Carboxyphenylamino)-4-((trans-4-(dimethylamino)cyclohexyl)amino)-5-nitropyrimidine 514831-13-1P, 2-(4-Carboxyphenylamino)-4-(trans-4-dimethylaminocyclohexylamino)-5-trifluoromethylpyrimidine 514831-20-0P, 2-(3,4-Dichlorophenylamino)-4-(trans-4-carboxycyclohexylamino)-5-trifluoromethylpyrimidine 514831-41-5P, 2-(3,4-Dichlorophenylamino)-4-(((4-(N,N-dimethylaminomethyl)cyclohexyl)methyl)amino)-5-trifluoromethylpyrimidine 514831-79-9P, 2-(3,4-Dichlorophenylamino)-4-(4-dimethylaminocyclohexylamino)-5-trifluoromethylpyrimidine 514832-17-8P, 2-(3,4-Dichlorophenylamino)-4-[(4-(2-carboxyethyl)cyclohexyl)amino]-5-trifluoromethylpyrimidine 514832-18-9P, 2-(4-Chlorophenylamino)-4-((trans-4-carboxycyclohexyl)amino)-5-nitropyrimidine 514832-54-3P, 2-(3,4-Dichlorophenylamino)-4-(3-carboxycyclohexylamino)-5-trifluoromethylpyrimidine 514832-61-2P, 2-(4-Chlorophenylamino)-4-(4-dimethylaminocyclohexylamino)-5-nitropyrimidine 514832-72-5P, 2-(4-Chlorophenylamino)-4-(3-carboxycyclohexylamino)-5-nitropyrimidine 514832-73-6P, 2-(4-Chlorophenylamino)-4-[(4-(2-carboxyethyl)cyclohexyl)amino]-5-nitropyrimidine 514832-78-1P, 2-(4-Chlorophenylamino)-4-(((4-

(N,N-dimethylaminomethyl)cyclohexyl)methyl)amino)-5-nitropyrimidine 514833-45-5P, 2-(3,4-Dichlorophenylamino)-4-[N-(4-methoxycarbonylcyclohexyl)-N-(3-pyridylmethyl)amino]-5-trifluoromethylpyrimidine 514834-33-4P, 2-(3,4-Dichlorophenylamino)-4-[(4-(3-carboxypropyl)cyclohexyl)amino]-5-trifluoromethylpyrimidine 514834-34-5P, 2-(3,4-Dichlorophenylamino)-4-[((4-(2-carboxyethyl)cyclohexyl)methyl)amino]-5-trifluoromethylpyrimidine 514834-50-5P, 2-(3,4-Dichlorophenylamino)-4-[((3-(tert-butoxycarbonylaminomethyl)cyclohexyl)methyl)amino]-5-trifluoromethylpyrimidine 514834-57-2P, 2-(3,4-Dichlorophenylamino)-4-(2-dimethylaminocyclohexylamino)-5-trifluoromethylpyrimidine 514835-37-1P, 2-(4-Chlorophenylamino)-4-(cis-4-carboxycyclohexylamino)-5-nitropyrimidine 514836-32-9P, 2-(4-Chlorophenylamino)-4-[((4-(2-carboxyethyl)cyclohexyl)methyl)amino]-5-nitropyrimidine 514836-51-2P, 2-(4-Chlorophenylamino)-4-[((3-((tert-butoxycarbonylamino)methyl)cyclohexyl)methyl)amino]-5-nitropyrimidine 514836-62-5P, 2-(4-Chlorophenylamino)-4-(2-dimethylaminocyclohexylamino)-5-nitropyrimidine 514837-09-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of trisubstituted pyrimidines as cyclin dependent kinase inhibitors)

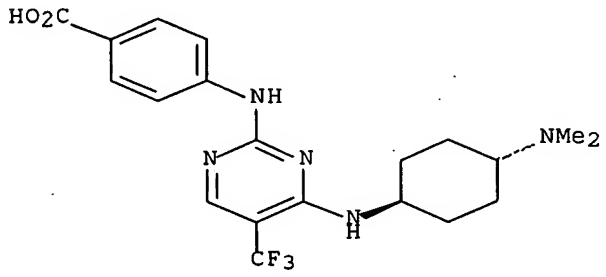
RN 514830-77-4 CAPLUS
CN Benzoic acid, 4-[[4-[[trans-4-(dimethylamino)cyclohexyl]amino]-5-nitro-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



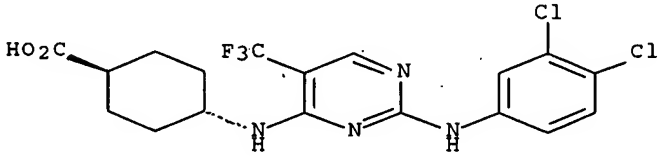
RN 514831-13-1 CAPLUS
CN Benzoic acid, 4-[[4-[[trans-4-(dimethylamino)cyclohexyl]amino]-5-(trifluoromethyl)-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

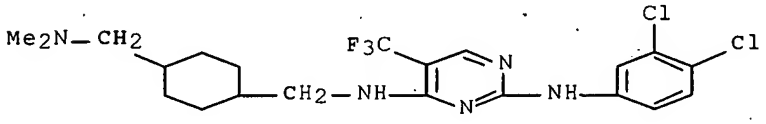


RN 514831-20-0 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]amino]-, trans- (9CI) (CA INDEX NAME)

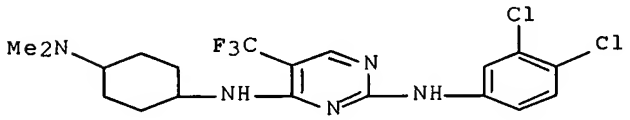
Relative stereochemistry.



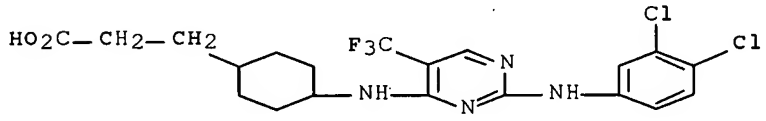
RN 514831-41-5 CAPLUS
CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-[[4-[(dimethylamino)methyl]cyclohexyl]methyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 514831-79-9 CAPLUS
CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-[4-(dimethylamino)cyclohexyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

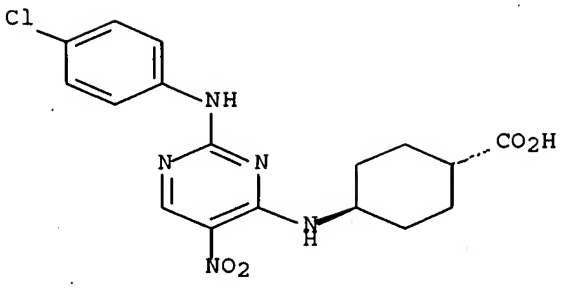


RN 514832-17-8 CAPLUS
CN Cyclohexanepropanoic acid, 4-[[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

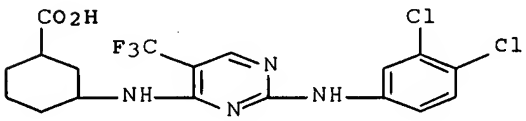


RN 514832-18-9 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-, trans- (9CI) (CA INDEX NAME)

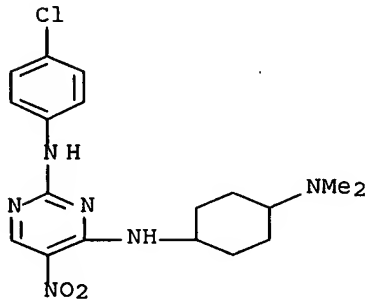
Relative stereochemistry.



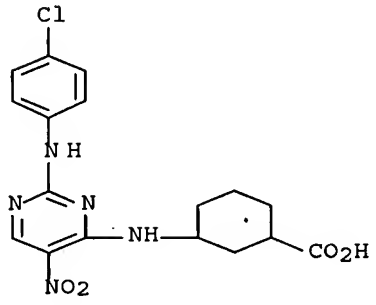
RN 514832-54-3 CAPLUS
CN Cyclohexanecarboxylic acid, 3-[[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



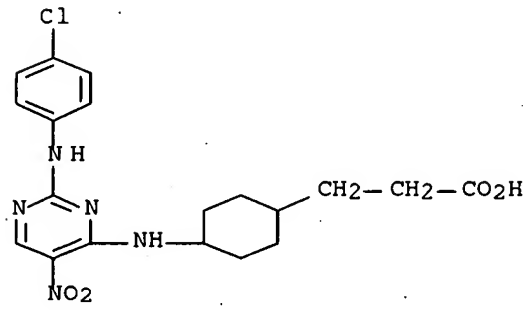
RN 514832-61-2 CAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[4-(dimethylamino)cyclohexyl]-5-nitro- (9CI) (CA INDEX NAME)



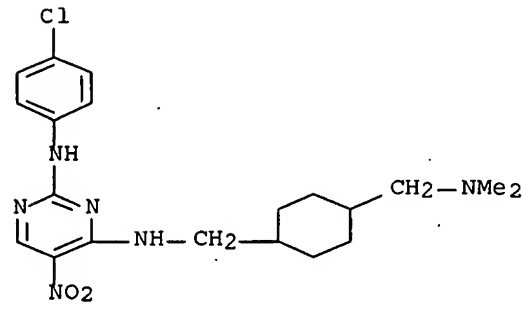
RN 514832-72-5 CAPLUS
CN Cyclohexanecarboxylic acid, 3-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



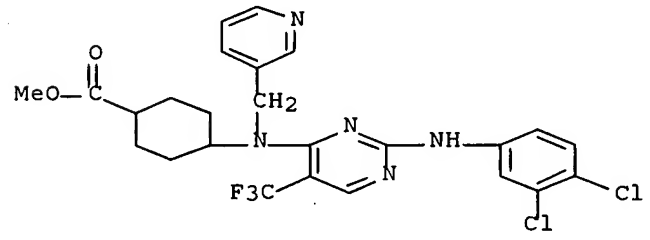
RN 514832-73-6 CAPLUS
CN Cyclohexanepropanoic acid, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



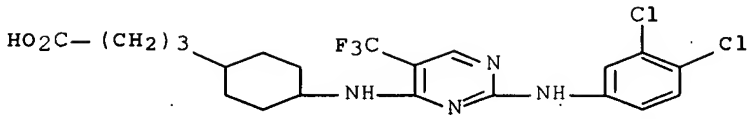
RN 514832-78-1 CAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[[4-[(dimethylamino)methyl]cyclohexyl]methyl]-5-nitro- (9CI) (CA INDEX NAME)



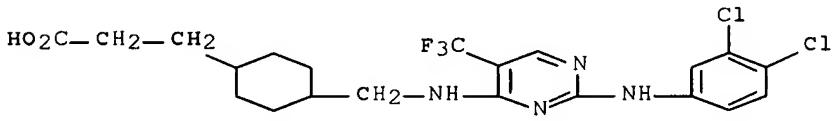
RN 514833-45-5 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl](3-pyridinylmethyl)amino]-, methyl ester (9CI) (CA INDEX NAME)



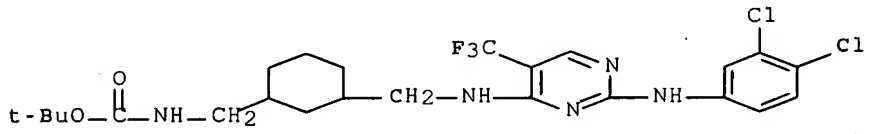
RN 514834-33-4 CAPLUS
CN Cyclohexanebutanoic acid, 4-[[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



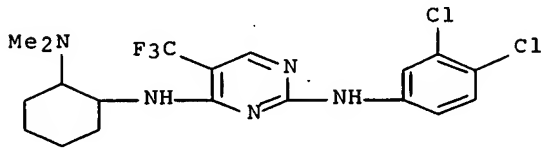
RN 514834-34-5 CAPLUS
CN Cyclohexanepropanoic acid, 4-[[[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)



RN 514834-50-5 CAPLUS
CN Carbamic acid, [[3-[[[2-[(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-4-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

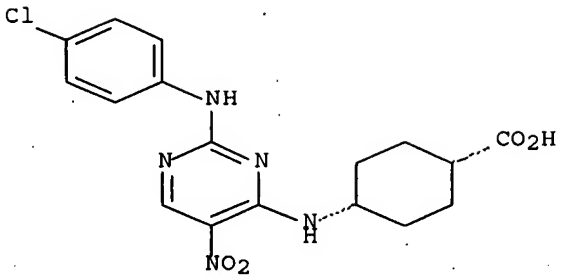


RN 514834-57-2 CAPLUS
CN 2,4-Pyrimidinediamine, N2-(3,4-dichlorophenyl)-N4-[2-(dimethylamino)cyclohexyl]-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

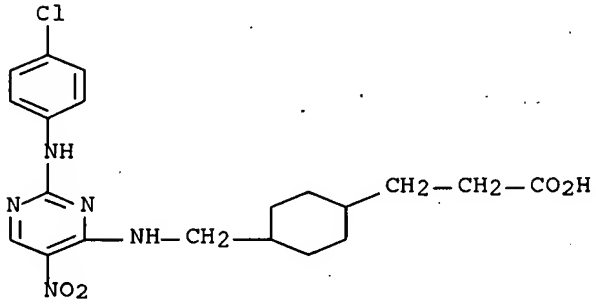


RN 514835-37-1 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]-, cis- (9CI) (CA INDEX NAME)

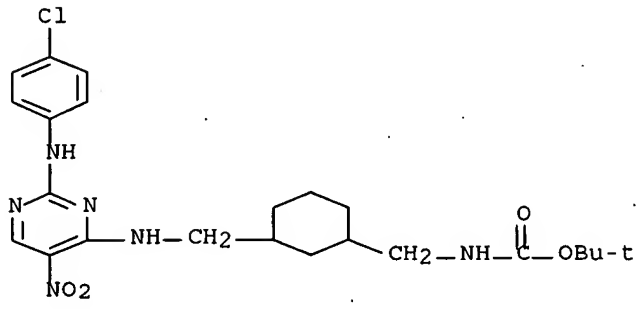
Relative stereochemistry.



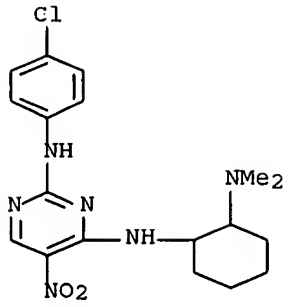
RN 514836-32-9 CAPLUS
CN Cyclohexanepropanoic acid, 4-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)



RN 514836-51-2 CAPLUS
CN Carbamic acid, [[3-[[[2-[(4-chlorophenyl)amino]-5-nitro-4-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

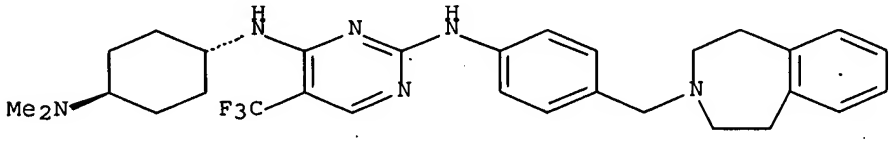


RN 514836-62-5 CAPLUS
CN 2,4-Pyrimidinediamine, N2-(4-chlorophenyl)-N4-[2-(dimethylamino)cyclohexyl]-5-nitro- (9CI) (CA INDEX NAME)



RN 514837-09-3 CAPLUS
CN 2,4-Pyrimidinediamine, N4-[trans-4-(dimethylamino)cyclohexyl]-N2-[4-[(1,2,4,5-tetrahydro-3H-3-benzazepin-3-yl)methyl]phenyl]-5-(trifluoromethyl)-, dihydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.



●2 HCl

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 15 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:927413 CAPLUS Full-text
DOCUMENT NUMBER: 138:14070
TITLE: CDK inhibiting pyrimidines
INVENTOR(S): Brumby, Thomas; Jautelat, Rolf; Prien, Olaf; Schaefer, Martina; Siemeister, Gerhard; Luecking, Ulrich; Huwe, Christoph
PATENT ASSIGNEE(S): Schering Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 240 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002096888	A1	20021205	WO 2002-EP5669	20020523 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,

BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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CA 2449118	A1	20021205	CA 2002-2449118	20020523	<--
AU 2002312933	A1	20021209	AU 2002-312933	20020523	<--
EP 1392662	A1	20040303	EP 2002-738100	20020523	<--

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BR 2002009774	A	20040601	BR 2002-9774	20020523	<--
JP 2004535414	T	20041125	JP 2003-500067	20020523	<--
CN 1633419	A	20050629	CN 2002-814886	20020523	<--
NZ 529654	A	20051223	NZ 2002-529654	20020523	<--
US 2004102630	A1	20040527	US 2002-156759	20020529	<--
US 7235561	B2	20070626			
IN 2003DN02240	A	20060120	IN 2003-DN2240	20031222	<--
US 2004224966	A1	20041111	US 2004-842419	20040511	<--
ZA 200309824	A	20060531	ZA 2003-9824	20060320	<--

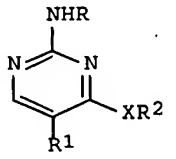
PRIORITY APPLN. INFO.:

DE 2001-10127581	A	20010529	<--
DE 2002-10212098	A	20020311	<--
WO 2002-EP5669	W	20020523	<--
US 2002-156759	A3	20020529	<--

OTHER SOURCE(S): MARPAT 138:14070

ED Entered STN: 06 Dec 2002

GI



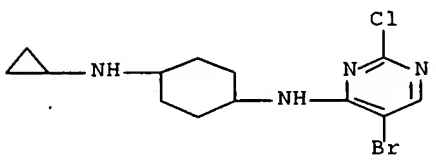
I

AB Pyrimidines I [R = (un)substituted Ph; R1 = H, halogen, (un)substituted alkyl, NO2, acyl, OCF3, SCF3, SO2CF3; R2 = (un)substituted alkyl, alkenyl, alkynyl; X = O, (un)substituted NH, cycloalkoxy; XR2 = (un)substituted cycloalkyl, heterocyclic] were prepared as inhibitors of the cyclin-dependent kinase. Thus, 2-chloro-4-propargylaminopyrimidine was treated with 4-F2CHSC6H4NH2.HCl to give I [X = NH, R = 4-F2CHSC6H4, R1 = Br, R2 = CH2C.tplbond.CH] which had IC50 for inhibition of CDK2 of 180 nM and for inhibition of MCF7 tumor cell proliferation of 3 μM.

IT 477593-38-7P 477593-41-2P 477593-42-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclin-dependent kinase inhibition of arylaminopyrimidines)

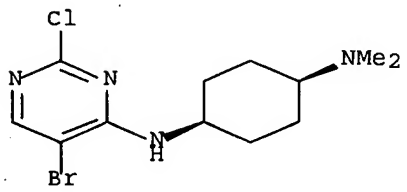
RN 477593-38-7 CAPLUS

CN 1,4-Cyclohexanediamine, N-(5-bromo-2-chloro-4-pyrimidinyl)-N'-cyclopropyl- (9CI) (CA INDEX NAME)



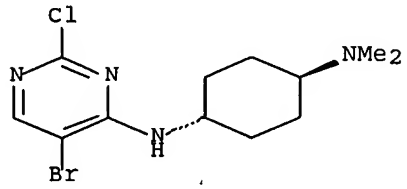
RN 477593-41-2 CAPLUS
CN 1,4-Cyclohexanediamine, N'-(5-bromo-2-chloro-4-pyrimidinyl)-N,N-dimethyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 477593-42-3 CAPLUS
CN 1,4-Cyclohexanediamine, N'-(5-bromo-2-chloro-4-pyrimidinyl)-N,N-dimethyl-, trans- (9CI) (CA INDEX NAME)

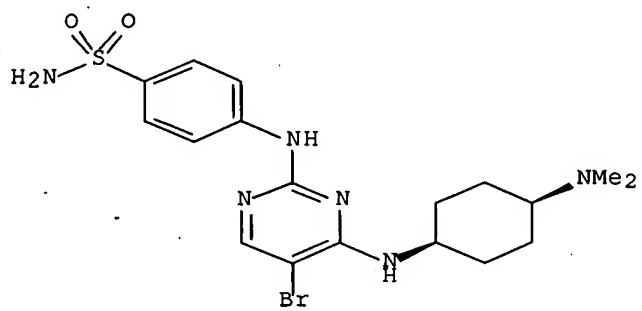
Relative stereochemistry.



IT 477589-08-5P 477589-09-6P 477589-12-1P
477589-16-5P 477589-17-6P 477589-48-3P
477589-49-4P 477589-51-8P 477589-52-9P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and cyclin-dependent kinase inhibition of arylaminopyrimidines)

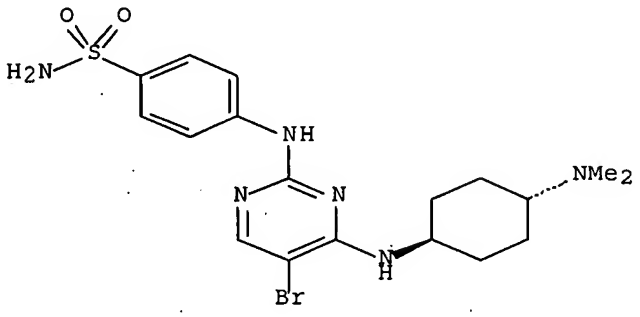
RN 477589-08-5 CAPLUS
CN Benzenesulfonamide, 4-[[5-bromo-4-[[cis-4-(dimethylamino)cyclohexyl]amino]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

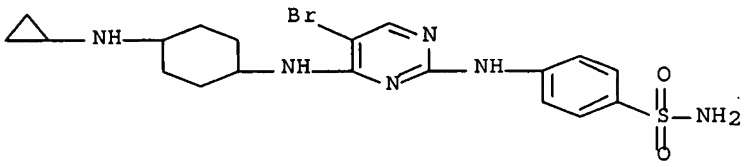


RN 477589-09-6 CAPLUS
CN Benzenesulfonamide, 4-[[5-bromo-4-[[trans-4-(dimethylamino)cyclohexyl]amino]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

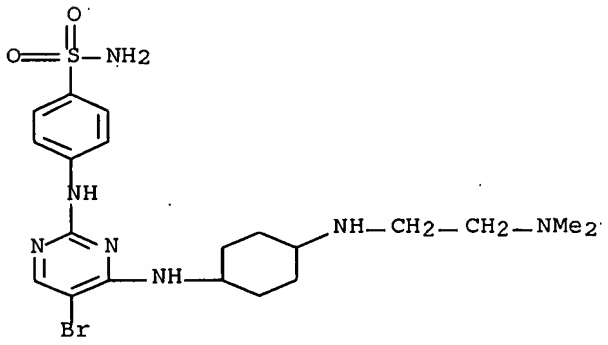
Relative stereochemistry.



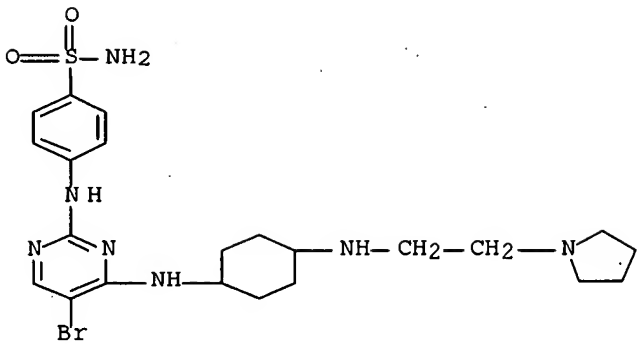
RN 477589-12-1 CAPLUS
CN Benzenesulfonamide, 4-[[5-bromo-4-[[4-(cyclopropylamino)cyclohexyl]amino]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



RN 477589-16-5 CAPLUS
CN Benzenesulfonamide, 4-[[5-bromo-4-[[4-[[2-(dimethylamino)ethyl]amino]cyclohexyl]amino]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

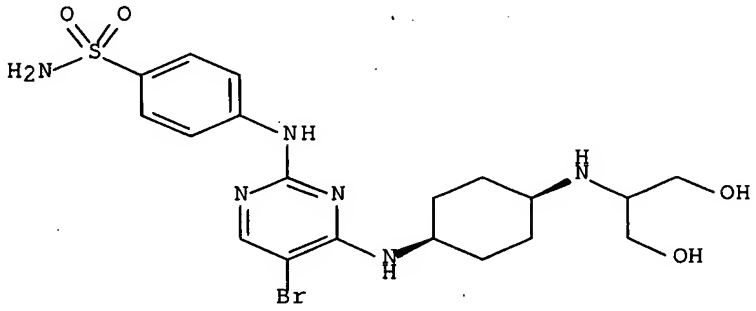


RN 477589-17-6 CAPLUS
CN Benzenesulfonamide, 4-[[5-bromo-4-[[4-[[2-(1-pyrrolidinyl)ethyl]amino]cyclohexyl]amino]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



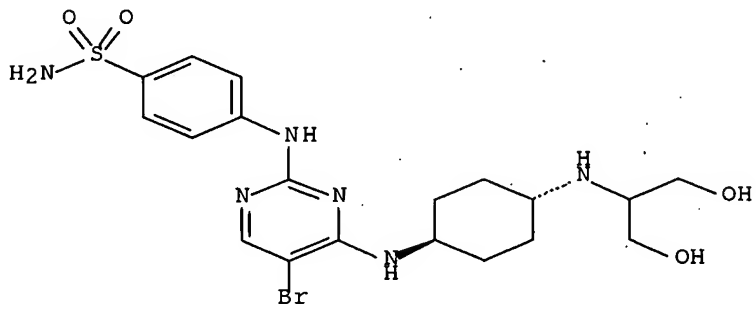
RN 477589-48-3 CAPLUS
CN Benzenesulfonamide, 4-[[5-bromo-4-[[cis-4-[[2-hydroxy-1-(hydroxymethyl)ethyl]amino]cyclohexyl]amino]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



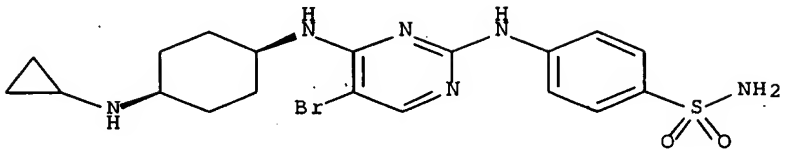
RN 477589-49-4 CAPLUS
CN Benzenesulfonamide, 4-[[5-bromo-4-[[trans-4-[[2-hydroxy-1-(hydroxymethyl)ethyl]amino]cyclohexyl]amino]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



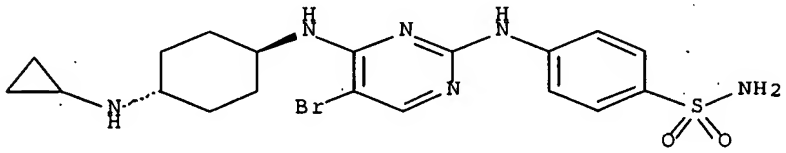
RN 477589-51-8 CAPLUS
CN Benzenesulfonamide, 4-[[5-bromo-4-[[cis-4-(cyclopropylamino)cyclohexyl]amino]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 477589-52-9 CAPLUS
CN Benzenesulfonamide, 4-[[5-bromo-4-[[trans-4-(cyclopropylamino)cyclohexyl]amino]-2-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

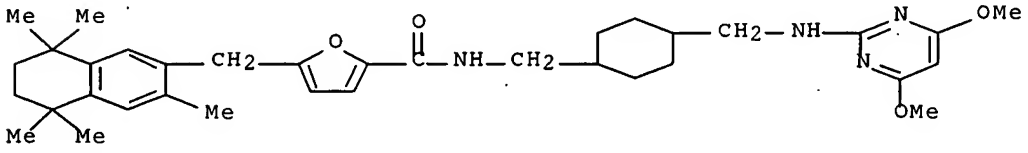


REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

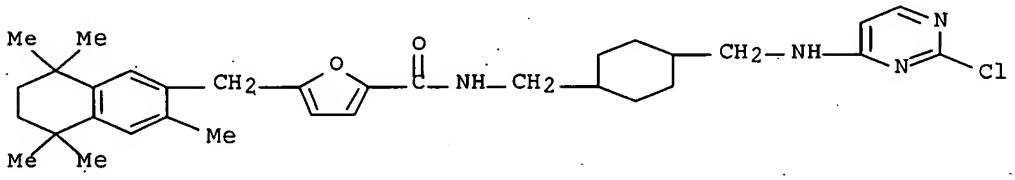
L23 ANSWER 16 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:878755 CAPLUS Full-text
DOCUMENT NUMBER: 139:17096
TITLE: Characterization of mono- and diaminopyrimidine derivatives as novel, nonpeptide gonadotropin releasing hormone (GnRH) receptor antagonists
AUTHOR(S): Luthin, David R.; Hong, Yufeng; Tompkins, Eileen; Anderes, Kenna L.; Paderes, Genevieve; Kraynov, Eugenia A.; Castro, Mary A.; Nared-Hood, Karen D.; Castillo, Rosemary; Gregory, Margaret; Vazir, Haresh; May, John M.; Anderson, Mark B.
CORPORATE SOURCE: Pfizer Global Research and Development-La Jolla/Agouron Pharmaceuticals, Inc., 10724 Science Center Drive, San Diego, CA, 92121, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(24), 3635-3639
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:17096
ED Entered STN: 20 Nov 2002
AB A novel series of derivs. of mono- and diaminopyrimidines 1 potently displaced binding of a radiolabeled GnRH analog to human and rat GnRH receptors. Analogs from these series competitively antagonized GnRH-stimulated increases in extracellular acidification in vitro and suppressed GnRH-mediated increases in circulating LH (LH) in castrated rats and testosterone in intact rats. These compds. or their analogs may be useful in treating sex hormone-dependent disease.
IT 263848-23-3P 263848-26-6P 263848-44-8P
263848-45-9P 263848-46-0P 263848-62-0P
263848-88-0P 263849-24-7P 263849-27-0P

537696-28-9P
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(characterization of mono- and diaminopyrimidine derivs. as novel, nonpeptide gonadotropin releasing hormone (GnRH) receptor antagonists)

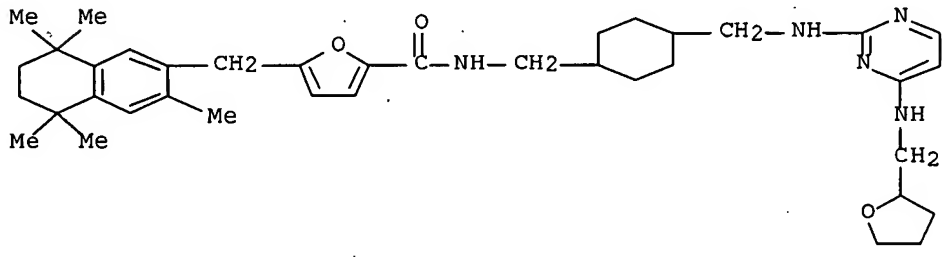
RN 263848-23-3 CAPLUS
CN 2-Furancarboxamide, N-[[4-[[(4,6-dimethoxy-2-pyrimidinyl)amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



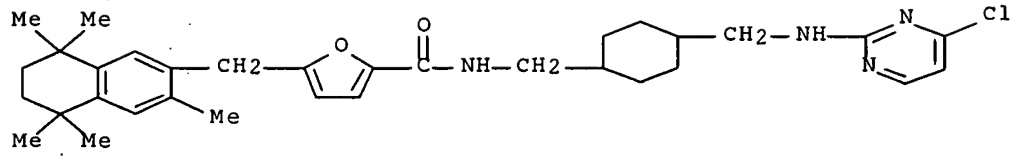
RN 263848-26-6 CAPLUS
CN 2-Furancarboxamide, N-[[4-[[(2-chloro-4-pyrimidinyl)amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



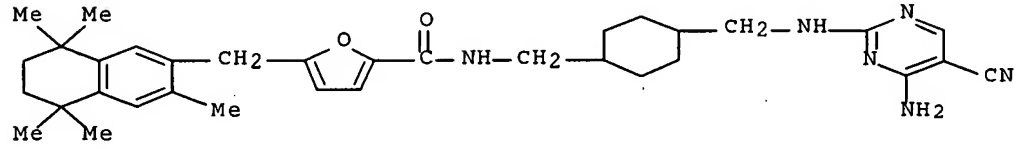
RN 263848-44-8 CAPLUS
CN 2-Furancarboxamide, N-[[4-[[[4-[[(tetrahydro-2-furanyl)methyl]amino]-2-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



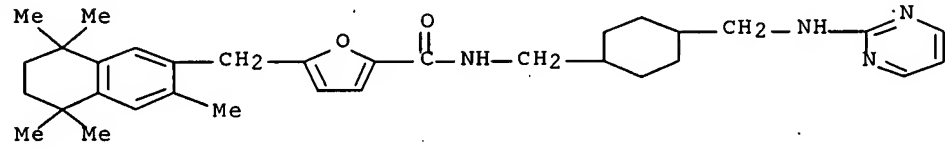
RN 263848-45-9 CAPLUS
CN 2-Furancarboxamide, N-[[4-[[(4-chloro-2-pyrimidinyl)amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



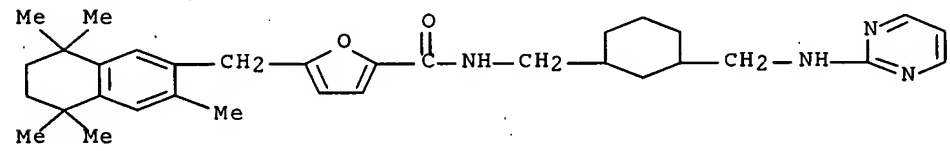
RN 263848-46-0 CAPLUS
CN 2-Furancarboxamide, N-[[4-[[(4-amino-5-cyano-2-pyrimidinyl)amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



RN 263848-62-0 CAPLUS
CN 2-Furancarboxamide, N-[[4-[(2-pyrimidinylamino)methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

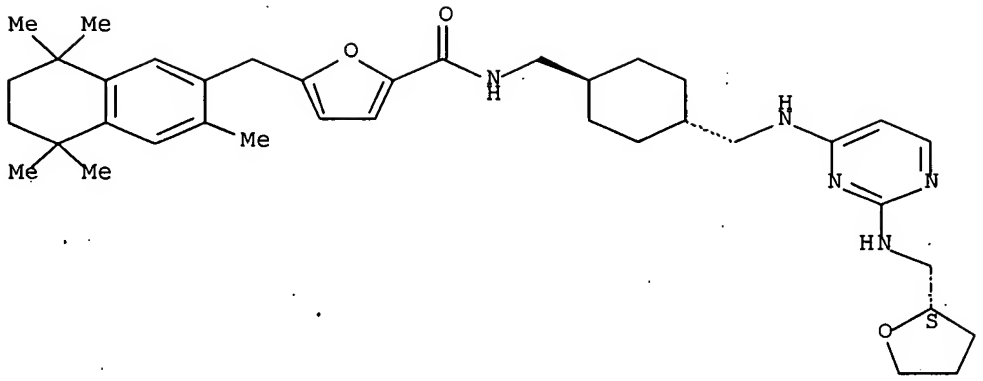


RN 263848-88-0 CAPLUS
CN 2-Furancarboxamide, N-[[3-[(2-pyrimidinylamino)methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



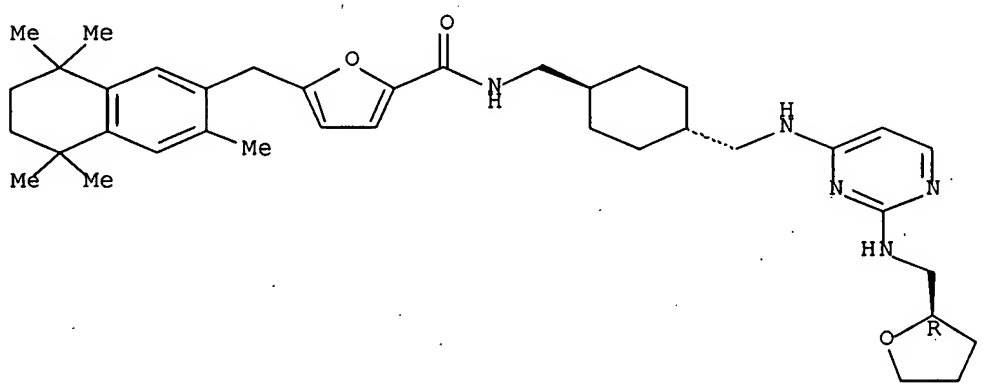
RN 263849-24-7 CAPLUS
CN 2-Furancarboxamide, N-[[trans-4-[[[2-[[[(2S)-tetrahydro-2-furanyl]methyl]amino]-4-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

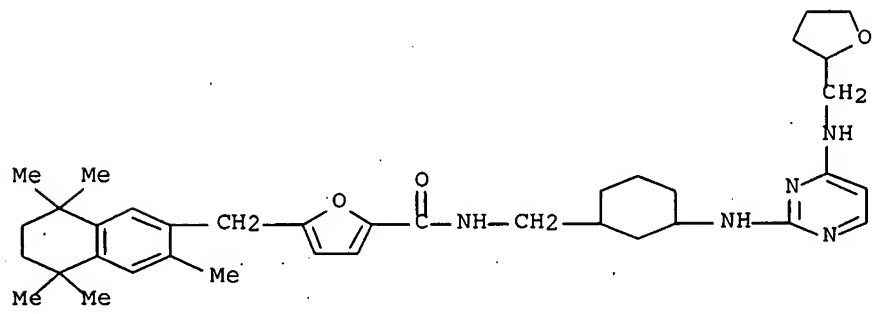


RN 263849-27-0 CAPLUS
CN 2-Furancarboxamide, N-[[trans-4-[[[2-[[[(2R)-tetrahydro-2-furanyl]methyl]amino]-4-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 537696-28-9 CAPLUS
CN 2-Furancarboxamide, N-[[3-[[4-[[(tetrahydro-2-furanyl)methyl]amino]-2-pyrimidinyl]amino]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 17 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:293616 CAPLUS Full-text
DOCUMENT NUMBER: 136:325560
TITLE: Preparation of aliphatic nitrogenous five-membered ring compounds as dipeptidyl peptidase IV inhibitors
INVENTOR(S): Yasuda, Kosuke; Morimoto, Hiroshi; Kawanami, Saburo; Hikota, Masataka; Matsumoto, Takeshi; Arakawa, Kenji
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: PCT Int. Appl., 164 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2002030891	A1	20020418	WO 2001-JP8803		20011005 <--
W: AE, AG, AL, AU, BA, BB, BG, BR, BZ, CA, CN, CO, CR, CU, CZ, DM, DZ, EC, EE, GD, GE, HR, HU, ID, IL, IN, IS, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NO, NZ, PH, PL, RO, SG, SI, SK, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 200194197	A	20020422	AU 2001-94197		20011005 <--
JP 2002356471	A	20021213	JP 2001-309558		20011005 <--
JP 2002356472	A	20021213	JP 2001-309559		20011005 <--
CA 2424600	A1	20030402	CA 2001-2424600		20011005 <--
BR 2001014436	A	20030701	BR 2001-14436		20011005 <--
EP 1325910	A1	20030709	EP 2001-974717		20011005 <--
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HU 200303391	A2	20040301	HU 2003-3391		20011005 <--
NZ 524974	A	20051028	NZ 2001-524974		20011005 <--
CN 1891689	A	20070110	CN 2006-10077863		20011005 <--
IN 2003KN00303	A	20050311	IN 2003-KN303		20030312 <--
ZA 2003002030	A	20030926	ZA 2003-2030		20030313 <--
NO 2003001490	A	20030602	NO 2003-1490		20030402 <--
US 2004063935	A1	20040401	US 2003-398486		20030404 <--
US 6849622	B2	20050201			
JP 2004035574	A	20040205	JP 2003-368572		20031029 <--
US 2004229926	A1	20041118	US 2004-872442		20040622 <--
US 7160877	B2	20070109			
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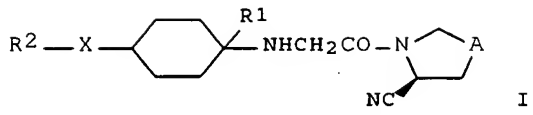
PRIORITY APPLN. INFO.:			JP 2000-308528	A	20001006 <--
			JP 2000-312562	A	20001012 <--
			JP 2001-99251	A	20010330 <--
			CN 2001-816674	A3	20011005 <--
			JP 2001-309558	A3	20011005 <--
			JP 2001-309559	A3	20011005 <--
			WO 2001-JP8803	W	20011005 <--
			US 2003-398486	A3	20030404

OTHER SOURCE(S): MARPAT 136:325560
ED Entered STN: 19 Apr 2002
GI



I

AB Aliphatic nitrogenous five-membered ring compds., (S)-N-(N-cyclohexylglycyl)pyrrolidine-2-carbonitrile and (R)-N-(N-cyclohexylglycyl)thiazolidine-2-carbonitrile, of the general formula (I) or pharmacol. acceptable salts thereof [wherein A is CH2 or S; R1 is hydrogen, lower alkyl, hydroxy-lower alkyl, or lower alkoxy-lower alkyl; X is N(R3), O, or CO; R3 is hydrogen or lower alkyl; and R2 is an optionally substituted mono- or bicyclic hydrocarbyl or heterocyclyl group or optionally substituted amino] are prepared These compds. are useful as dipeptidyl peptidase IV inhibitors for the prevention or treatment of diabetes, in particular type II diabetes (no data). Thus, a solution of (S)-1-bromoacetyl-2-cyanopyrrolidine and N-(5-nitro-2-pyridyl)-trans-1,4- cyclohexanediamine in MeOH/MeCN was stirred at room temperature for 15 h to give, after treatment with 2 N HCl/Et2O in EtOAc/CHCl3, (S)-2-cyano-1-[[[trans-4-(5-nitro-2-pyridylamino)cyclohexyl]amino]acetyl]p yrrolidine dihydrochloride.

IT 412284-89-0P 412284-90-3P 412284-91-4P
412284-92-5P 412285-02-0P 412285-03-1P
412285-05-3P 412285-08-6P 412285-09-7P
412285-11-1P 412285-12-2P 412285-13-3P
412285-14-4P 412285-15-5P 412285-16-6P
412285-17-7P 412285-18-8P 412285-19-9P
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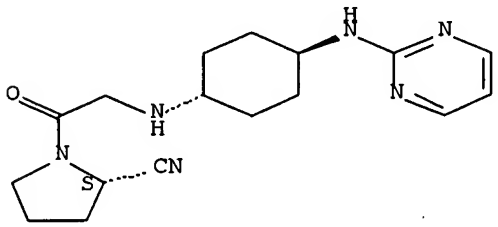
412285-64-4P 412285-65-5P 412288-75-6P
412288-76-7P 412288-77-8P 412288-78-9P
412915-48-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (S)-N-(N-cyclohexylglycyl)pyrrolidine-2-carbonitriles and (R)-N-(N-cyclohexylglycyl)thiazolidine-2-carbonitriles as dipeptidyl peptidase IV inhibitors for prevention or treatment of diabetes)

RN 412284-89-0 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-(2-pyrimidinylamino)cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

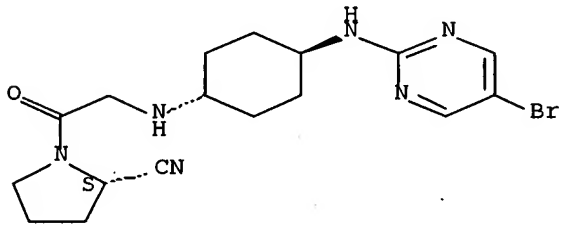
Absolute stereochemistry.



●2 HCl

RN 412284-90-3 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-bromo-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

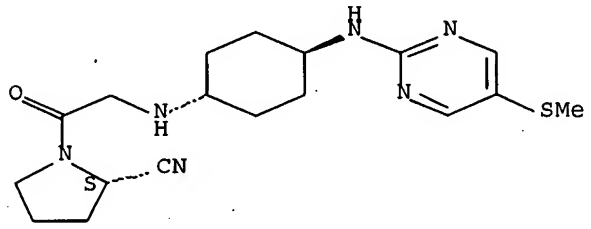
Absolute stereochemistry.



●2 HCl

RN 412284-91-4 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[5-(methylthio)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

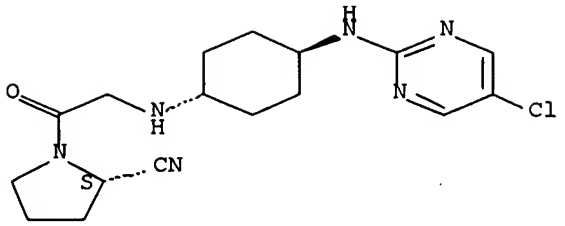
Absolute stereochemistry.



●2 HCl

RN 412284-92-5 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-chloro-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

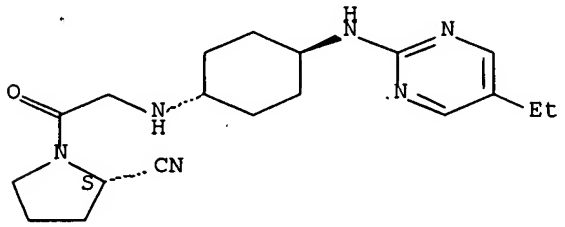
Absolute stereochemistry.



●2 HCl

RN 412285-02-0 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-ethyl-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

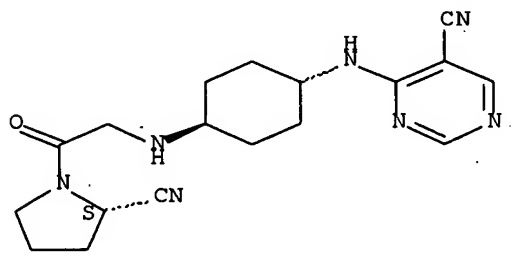
Absolute stereochemistry.



●2 HCl

RN 412285-03-1 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-cyano-4-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

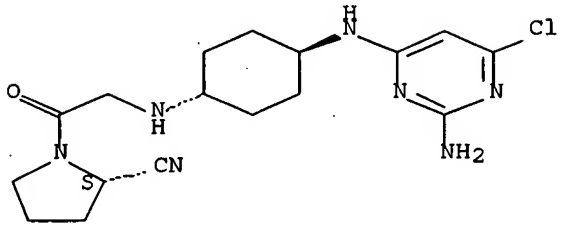
Absolute stereochemistry.



●2 HCl

RN 412285-05-3 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(2-amino-6-chloro-4-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

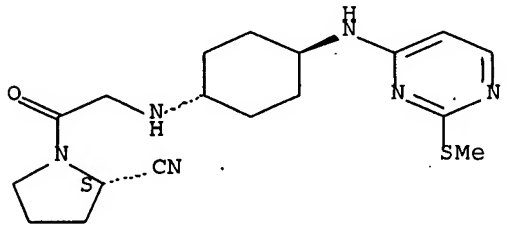
Absolute stereochemistry.



●2 HCl

RN 412285-08-6 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[2-(methylthio)-4-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

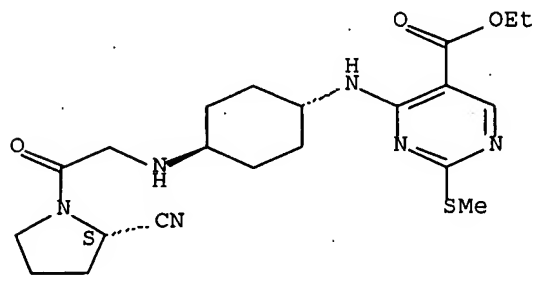
Absolute stereochemistry.



●2 HCl

RN 412285-09-7 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(methylthio)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

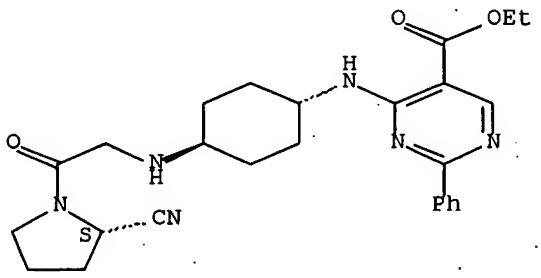
Absolute stereochemistry.



●2 HCl

RN 412285-11-1 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-phenyl-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

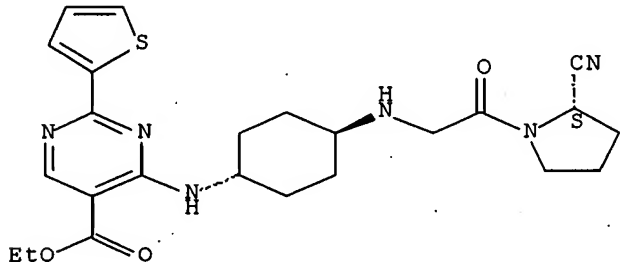
Absolute stereochemistry.



●2 HCl

RN 412285-12-2 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(2-thienyl)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

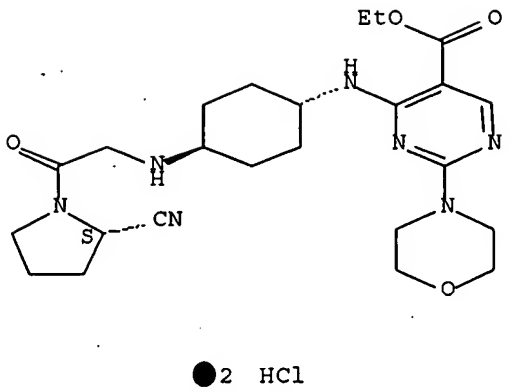
Absolute stereochemistry.



●2 HCl

RN 412285-13-3 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(4-morpholinyl)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

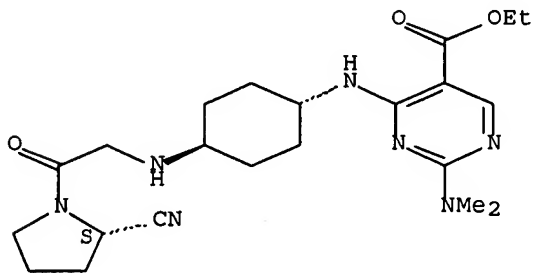
Absolute stereochemistry.



●2 HCl

RN 412285-14-4 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(dimethylamino)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

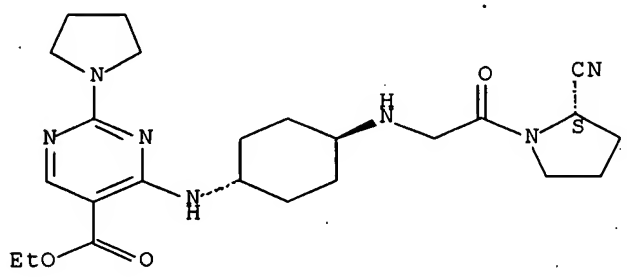
Absolute stereochemistry.



●2 HCl

RN 412285-15-5 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(1-pyrrolidinyl)-, ethyl ester, dihydrochloride (9CI) (CA INDEX NAME)

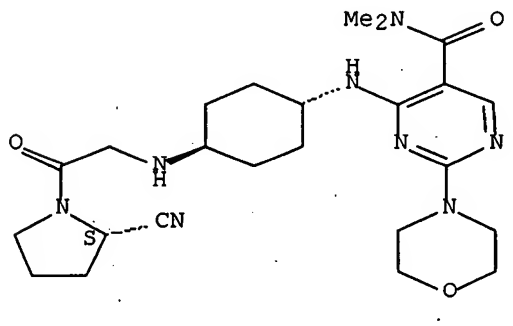
Absolute stereochemistry.



●2 · HCl

RN 412285-16-6 CAPLUS
CN 5-Pyrimidinecarboxamide, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-N,N-dimethyl-2-(4-morpholinyl)-, dihydrochloride (9CI) (CA INDEX NAME)

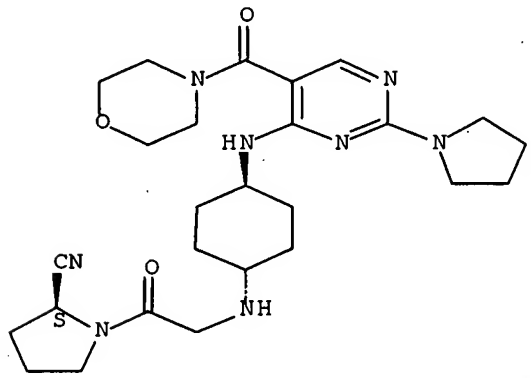
Absolute stereochemistry.



●2 HCl

RN 412285-17-7 CAPLUS
CN Morpholine, 4-[[4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(1-pyrrolidinyl)-5-pyrimidinyl]carbonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

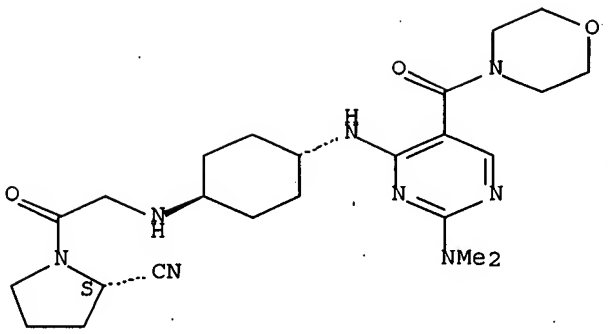
Absolute stereochemistry.



●2 HCl

RN 412285-18-8 CAPLUS
CN Morpholine, 4-[[4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(dimethylamino)-5-pyrimidinyl]carbonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

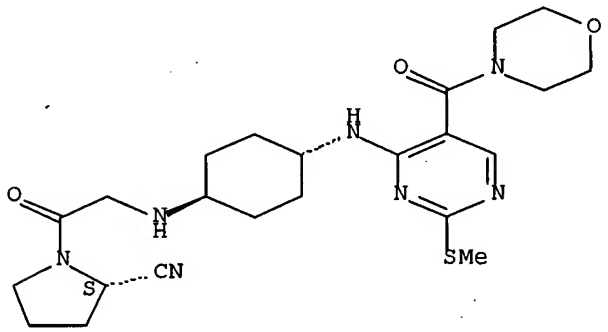
Absolute stereochemistry.



●2 HCl

RN 412285-19-9 CAPLUS
CN Morpholine, 4-[[4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-(methylthio)-5-pyrimidinyl]carbonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

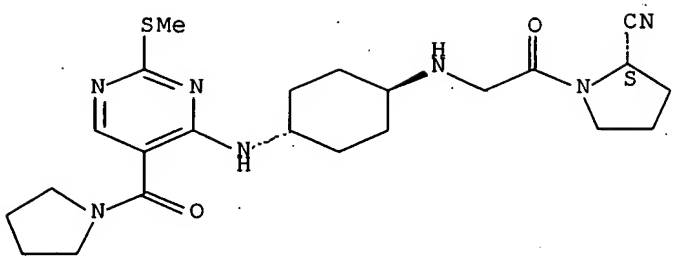
Absolute stereochemistry.



●2 HCl

RN 412285-20-2 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[2-(methylthio)-5-(1-pyrrolidinylcarbonyl)-4-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

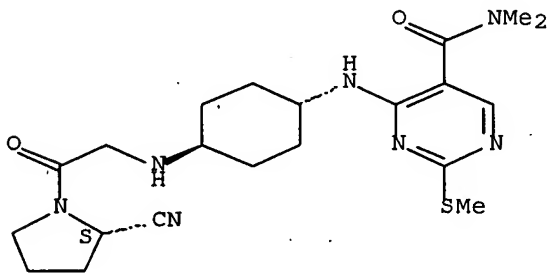
Absolute stereochemistry.



●2 HCl

RN 412285-21-3 CAPLUS
CN 5-Pyrimidinecarboxamide, 4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-N,N-dimethyl-2-(methylthio)-, dihydrochloride (9CI) (CA INDEX NAME)

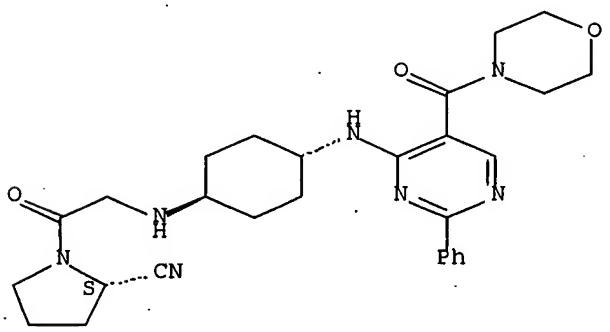
Absolute stereochemistry.



●2 HCl

RN 412285-22-4 CAPLUS
CN Morpholine, 4-[[4-[[trans-4-[[2-[(2S)-2-cyano-1-pyrrolidinyl]-2-oxoethyl]amino]cyclohexyl]amino]-2-phenyl-5-pyrimidinyl]carbonyl]-, dihydrochloride (9CI) (CA INDEX NAME)

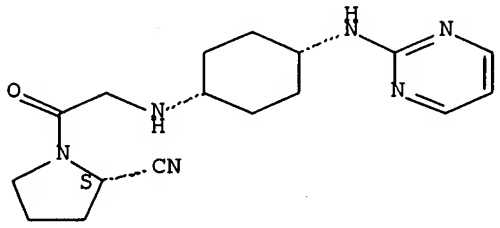
Absolute stereochemistry.



●2 HCl

RN 412285-43-9 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[cis-4-(2-pyrimidinylamino)cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

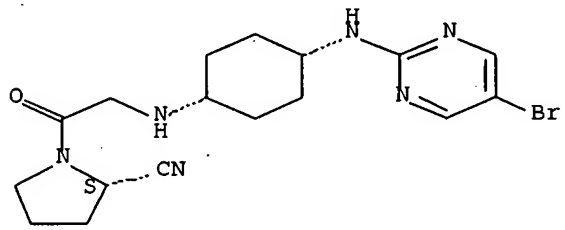
Absolute stereochemistry.



●2 HCl

RN 412285-44-0 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[cis-4-[(5-bromo-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

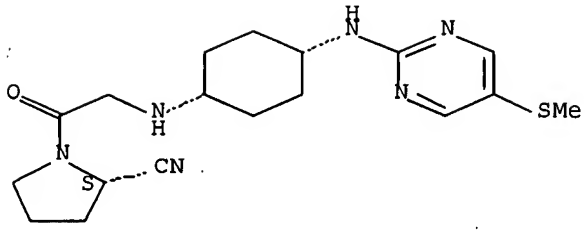
Absolute stereochemistry.



●2 HCl

RN 412285-45-1 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[cis-4-[[5-(methylthio)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

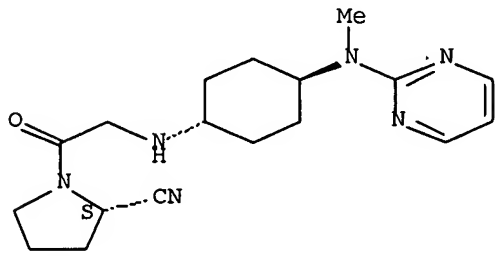
Absolute stereochemistry.



●2 HCl

RN 412285-64-4 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-(methyl-2-pyrimidinylamino)cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

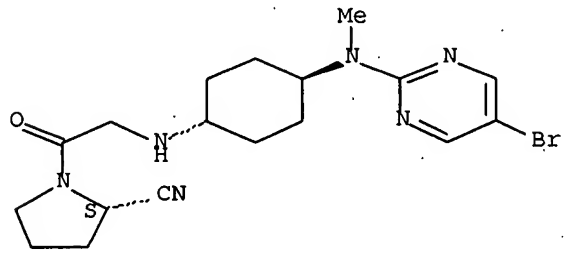
Absolute stereochemistry.



●2 HCl

RN 412285-65-5 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(5-bromo-2-pyrimidinyl)methylamino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

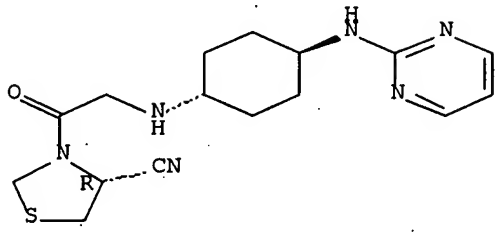
Absolute stereochemistry.



●2 HCl

RN 412288-75-6 CAPLUS
CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-(2-pyrimidinylamino)cyclohexyl]amino]acetyl]-, monohydrochloride, (4R)- (9CI) (CA INDEX NAME)

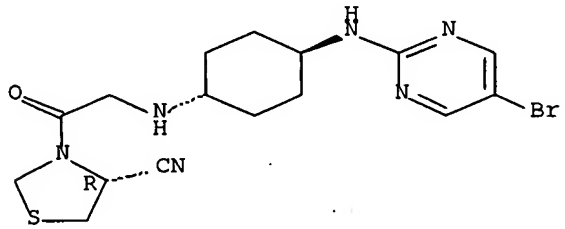
Absolute stereochemistry.



● HCl

RN 412288-76-7 CAPLUS
CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[(5-bromo-2-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

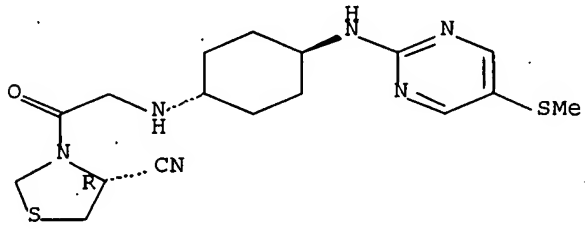
Absolute stereochemistry.



●2 HCl

RN 412288-77-8 CAPLUS
CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[[5-(methylthio)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

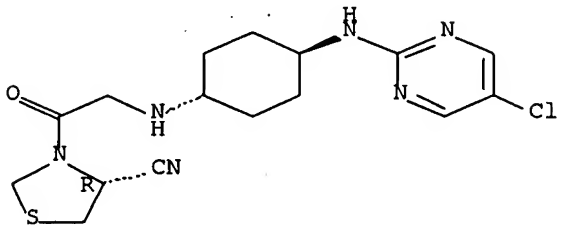


●2 HCl

RN 412288-78-9 CAPLUS
CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[(5-chloro-2-

pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

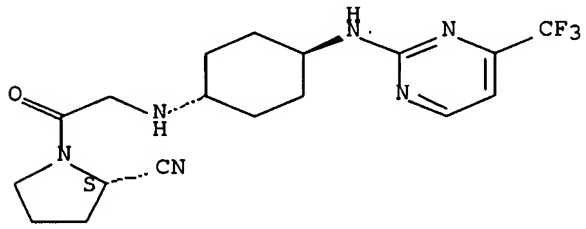
Absolute stereochemistry.



●2 HCl

RN 412915-48-1 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[4-(trifluoromethyl)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

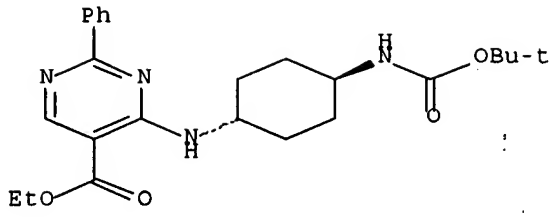
Absolute stereochemistry.



●2 HCl

IT 412294-04-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (S)-N-(N-cyclohexylglycyl)pyrrolidine-2-carbonitriles and (R)-N-(N-cyclohexylglycyl)thiazolidine-2-carbonitriles as dipeptidyl peptidase IV inhibitors for prevention or treatment of diabetes)
RN 412294-04-3 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 4-[[trans-4-[[(1,1-dimethylethoxy)carbonyl]amino]cyclohexyl]amino]-2-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



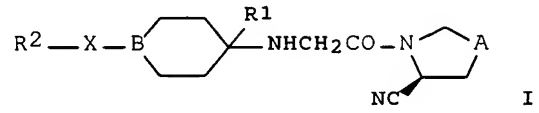
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 18 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:293615 CAPLUS Full-text
DOCUMENT NUMBER: 136:325559
TITLE: Preparation of nitrogenous five-membered ring compounds such as (S)-N-[N-cyclohexyl or N-(4-piperidinyl)glycyl]pyrrolidine-2-carbonitrile derivatives as dipeptidyl peptidase IV inhibitors
INVENTOR(S): Yasuda, Kosuke; Morimoto, Hiroshi; Kawanami, Saburo; Hikota, Masataka; Matsumoto, Takeshi; Arakawa, Kenji
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan
SOURCE: PCT Int. Appl., 117 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002030890	A1	20020418	WO 2001-JP8802	20011005 <--
W: AE, AG, AL, AU, BA, BB, BG, BR, BZ, CA, CN, CO, CR, CU, CZ, DM, DZ, EC, EE, GD, GE, HR, HU, ID, IL, IN, IS, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NO, NZ, PH, PL, RO, SG, SI, SK, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2424964	A1	20020418	CA 2001-2424964	20011005 <--
AU 200194196	A	20020422	AU 2001-94196	20011005 <--
JP 2002356471	A	20021213	JP 2001-309558	20011005 <--
JP 2002356472	A	20021213	JP 2001-309559	20011005 <--
EP 1323710	A1	20030702	EP 2001-974716	20011005 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
CN 1468216	A	20040114	CN 2001-816674	20011005 <--
NZ 525630	A	20041029	NZ 2001-525630	20011005 <--
CN 1891689	A	20070110	CN 2006-10077863	20011005 <--
ZA 2003002030	A	20030926	ZA 2003-2030	20030313 <--
US 2005054678	A1	20050310	US 2003-398485	20030404 <--
US 7138397	B2	20061121		
JP 2004035574	A	20040205	JP 2003-368572	20031029 <--
AU 2004237882	A1	20050106	AU 2004-237882	20041213 <--
JP 2005200427	A	20050728	JP 2005-105732	20050401 <--
AU 2005229666	A1	20051124	AU 2005-229666	20051102 <--
US 2006241146	A1	20061026	US 2006-452923	20060615 <--
PRIORITY APPLN. INFO.:			JP 2000-308528 A	20001006 <--

JP 2000-312562	A	20001012 <--
JP 2001-99251	A	20010330 <--
AU 2001-94196	A3	20011005 <--
CN 2001-816674	A3	20011005 <--
JP 2001-309558	A3	20011005 <--
JP 2001-309559	A3	20011005 <--
WO 2001-JP8802	W	20011005 <--
US 2003-398485	A3	20030404

OTHER SOURCE(S): MARPAT 136:325559
ED Entered STN: 19 Apr 2002
GI



I

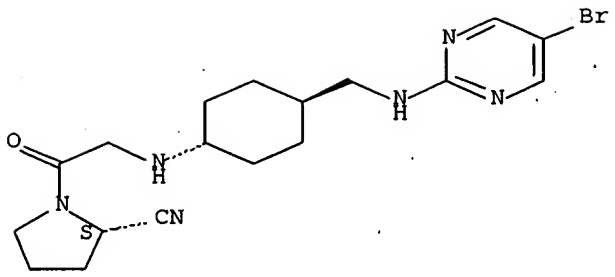
AB Aliphatic nitrogenous five-membered ring compds. of the general formula (I) or pharmacol. acceptable salts thereof [wherein A is CH2 or S; B is CH or N; R1 is H, lower alkyl, hydroxy-lower alkyl, lower alkoxy-lower alkyl; X is a single bond, CO, -Alk-CO-, -COCH2-, -Alk-O-, -O-CH2-, SO2, S, CO2, -CON(R3)-, -Alk-CON(R3)-, -CON(R3)CH2-, -Alk-CON(R3)CH2-, -COCH2N(R3)-, -SO2NR3-, or NHCH2; R3 is H or lower alkyl; Alk is lower alkylene; and R2 is (1) an optionally substituted mono or bicyclic hydrocarbyl or heterocyclyl, (2) amino substituted by 1- 2 of optionally substituted lower alkyl, or (3) lower alkyl, carboxy-lower alkyl, lower alkoxy, lower alkenyl, lower alkoxy-lower alkyl, PhO, phenoxy-lower alkyl, or phenyl-lower alkenyl with the proviso that when X is CO, B is N; or when X is a single bond, R2 is selected from groups listed in (1) and (2)] are prepared These compds. are useful as dipeptidyl peptidase IV inhibitors for the prevention or treatment of diabetes, in particular type II diabetes (no data). Thus, a solution of 100 mg (S)-1-bromoacetyl-2-cyanopyrrolidine and 247 mg 4-amino-1-(2-pyrimidinyl)piperidine in MeOH/MeCN was stirred at room temperature for 15 h to give, after treatment with 2 N HCl/Et2O, (S)-2-cyano-1-[[[1-(2-pyrimidinyl)piperidin-4-yl]amino]acetyl]pyrrolidine dihydrochloride.

IT 412355-56-7P 412355-59-0P 412355-60-3P
412355-61-4P 412355-75-0P 412355-76-1P
412355-77-2P 412355-78-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitrogenous five-membered ring compds. such as (S)-N-glycylpyrrolidinecarbonitrile derivs. as dipeptidyl peptidase IV inhibitors for prevention or treatment of diabetes, in particular type II diabetes)

RN 412355-56-7 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[(5-bromo-2-pyrimidinyl)amino]methyl]cyclohexyl]amino]acetyl]-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

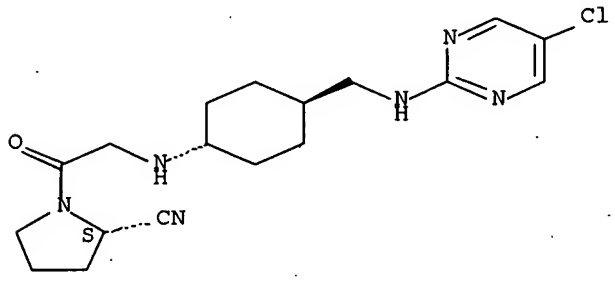
Absolute stereochemistry.



● HCl

RN 412355-59-0 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[(5-chloro-2-pyrimidinyl)amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI) (CA INDEX NAME)

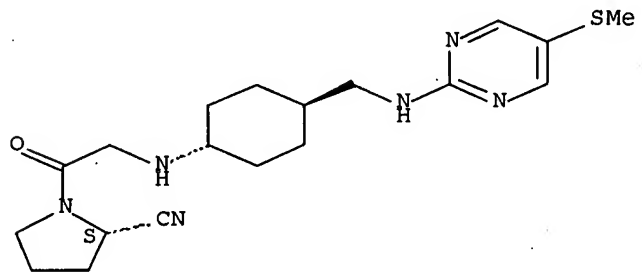
Absolute stereochemistry.



●2 HCl

RN 412355-60-3 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[[5-(methylthio)-2-pyrimidinyl]amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)-(9CI) (CA INDEX NAME)

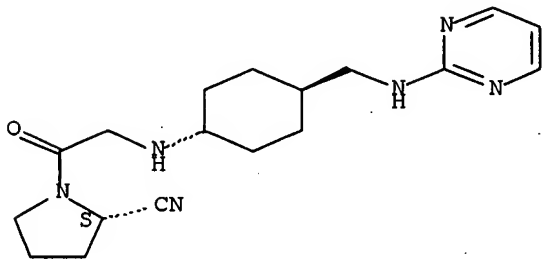
Absolute stereochemistry.



●2 HCl

RN 412355-61-4 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[(2-pyrimidinylamino)methyl]cycloh exyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

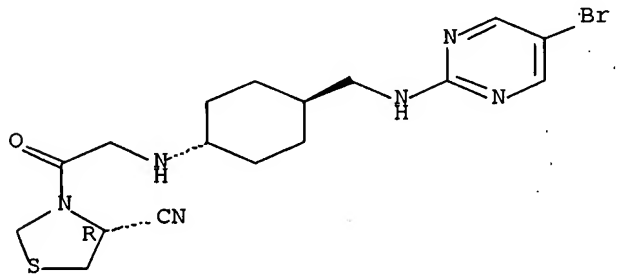
Absolute stereochemistry.



●2 HCl

RN 412355-75-0 CAPLUS
CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[[(5-bromo-2-pyrimidinyl)amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

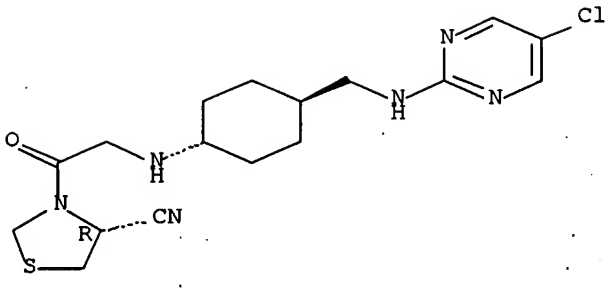
Absolute stereochemistry.



●2 HCl

RN 412355-76-1 CAPLUS
CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[[(5-chloro-2-pyrimidinyl)amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

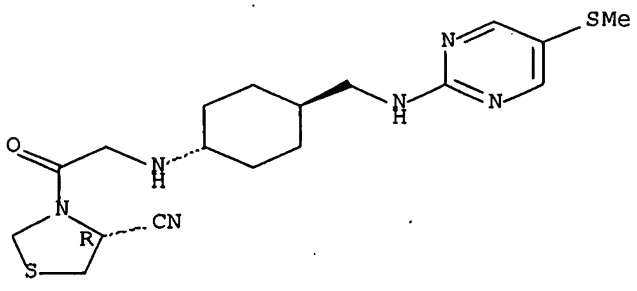
Absolute stereochemistry.



●2 HCl

RN 412355-77-2 CAPLUS
CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[[[5-(methylthio)-2-pyrimidinyl]amino]methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

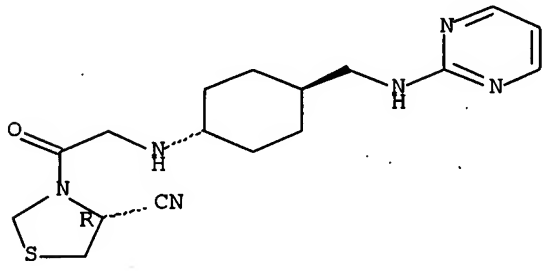
Absolute stereochemistry.



●2 HCl

RN 412355-78-3 CAPLUS
CN 4-Thiazolidinecarbonitrile, 3-[[[trans-4-[(2-pyrimidinylamino)methyl]cyclohexyl]amino]acetyl]-, dihydrochloride, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

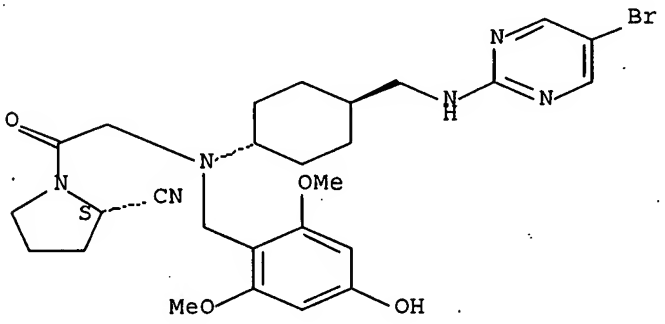


●2 HCl

IT 412357-15-4DP, resin-bound 412357-18-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitrogenous five-membered ring compds. such as (S)-N-glycylpyrrolidinecarbonitrile derivs. as dipeptidyl peptidase IV inhibitors for prevention or treatment of diabetes, in particular type II diabetes)

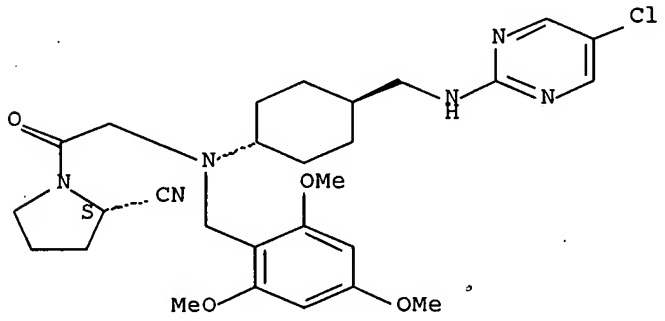
RN 412357-15-4 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[(5-bromo-2-pyrimidinyl)amino]methyl]cyclohexyl][(4-hydroxy-2,6-dimethoxyphenyl)methyl]amino]acetyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 412357-18-7 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[trans-4-[[(5-chloro-2-pyrimidinyl)amino]methyl]cyclohexyl][(2,4,6-trimethoxyphenyl)methyl]amino]acetyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

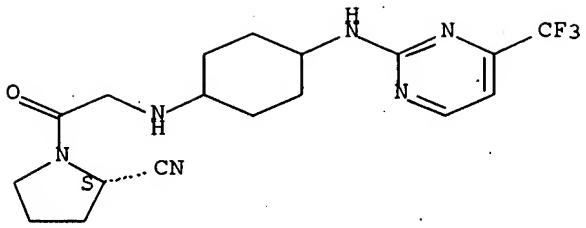
L23 ANSWER 19 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:923757 CAPLUS Full-text
DOCUMENT NUMBER: 136:37503
TITLE: Preparation of N-glycyl-2-cyanopyrrolidines as DPP IV inhibitors
INVENTOR(S): Villhauer, Edwin Bernard
PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis-Erfindungen Verwaltungsgesellschaft m.b.H.
SOURCE: PCT Int. Appl., 50 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2001096295	A2	20011220	WO 2001-EP6595		20010611 <--
WO 2001096295	A3	20020516			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
TW 583185	B	20040411	TW 2001-90113972		20010608 <--
CA 2411778	A1	20011220	CA 2001-2411778		20010611 <--
EP 1296974	A2	20030402	EP 2001-984014		20010611 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2004503531	T	20040205	JP 2002-510439		20010611 <--
US 6432969	B1	20020813	US 2001-879654		20010612 <--
US 2002193390	A1	20021219	US 2002-176440		20020620 <--
PRIORITY APPLN. INFO.:			US 2000-325743P	P	20000613 <--
			US 2000-592336	A	20000613 <--
			WO 2001-EP6595	W	20010611 <--
			US 2001-879654	A3	20010612 <--

OTHER SOURCE(S): MARPAT 136:37503
ED Entered STN: 21 Dec 2001
AB The present invention relates to the preparation of N-(substituted glycyl)-2-cyanopyrrolidines. Thus, 1-chloroacetyl-2-(S)-cyanopyrrolidine (synthetic preparation given) is reacted with 2-[(5-chloro-2-pyridinyl)amino]-1,1-dimethylethylamine in the presence of K2CO3 to give 1-[[[2-[(5-chloro-2-pyridinyl)amino]-1,1-dimethylethyl]amino]acetyl]-2- cyano-(S)-pyrrolidine. The prepared compds. inhibit DPP-IV (dipeptidyl-peptidase-IV) activity. They are therefore indicated for use as pharmaceuticals in inhibiting DPP-IV and in the treatment of conditions mediated by DPP-IV, such as non-insulin-dependent diabetes mellitus, arthritis, obesity, osteoporosis and further conditions of impaired glucose tolerance. Data for biol. activity of some of the prepared compds. were given.
IT 380831-65-2P 380831-69-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-glycyl-2-cyanopyrrolidines as DPP IV inhibitors)
RN 380831-65-2 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[4-[[4-(trifluoromethyl)-2-pyrimidinyl]amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

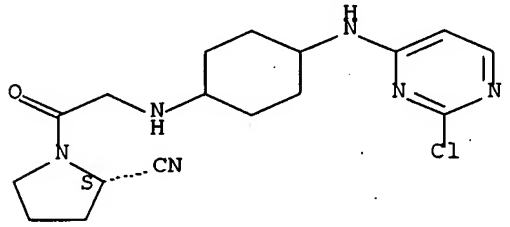
Absolute stereochemistry.



●2 HCl

RN 380831-69-6 CAPLUS
CN 2-Pyrrolidinecarbonitrile, 1-[[[4-[(2-chloro-4-pyrimidinyl)amino]cyclohexyl]amino]acetyl]-, dihydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



●2 HCl

L23 ANSWER 20 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:900621 CAPLUS Full-text
DOCUMENT NUMBER: 134:56683
TITLE: Preparation of nitrogen-containing heterocyclic derivatives as remedies for complications of diabetes based on protein kinase C inhibition
INVENTOR(S): Suzuki, Takayuki; Onda, Kenichi; Murakami, Takeshi; Negoro, Kenji; Yahiro, Kiyoshi; Maruyama, Tatsuya; Shimaya, Akiyoshi; Ohta, Mitsuaki
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000076980	A1	20001221	WO 2000-JP3768	20000609 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU,

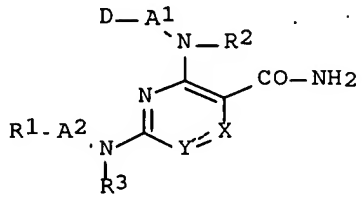
ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: JP 1999-163344 A 19990610 <--
JP 1999-165217 A 19990611 <--

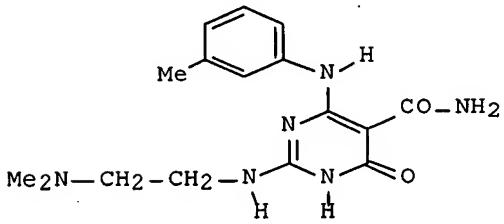
OTHER SOURCE(S): MARPAT 134:56683

ED Entered STN: 22 Dec 2000.

GI



I



II

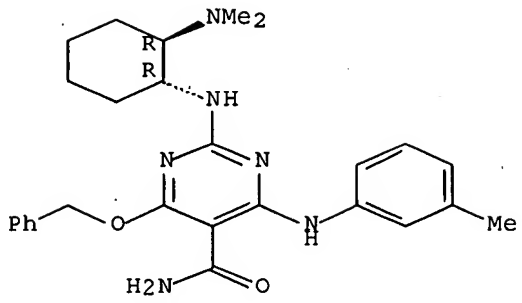
AB The title compds. I [Y and X together are N:N, C(R4):N, etc.; D = (un)substituted aryl, etc.; R1 = (un)substituted heteroaryl, etc.; A1, A2 = (un)substituted alkylene, etc.; R2, R3, R4 = H, OH, etc.; or R1A2NR3 = (un)substituted heteroaryl] are prepared The title compound II in vitro showed IC50 of 0.0049 μmol against protein kinase C.

IT 313337-98-3P 313337-99-4P 313338-14-6P
313338-15-7P 313338-42-0P 313338-55-5P
313338-56-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of nitrogen-containing heterocyclic derivs. as remedies for complications of diabetes)

RN 313337-98-3 CAPLUS

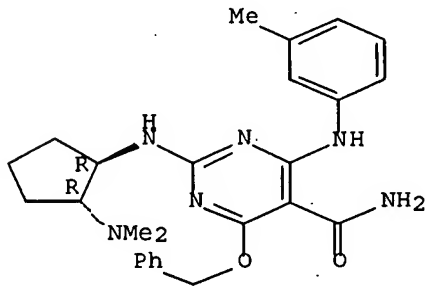
CN 5-Pyrimidinecarboxamide, 2-[[(1R,2R)-2-(dimethylamino)cyclohexyl]amino]-4-[(3-methylphenyl)amino]-6-(phenylmethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



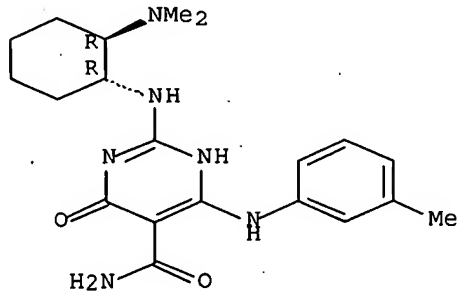
RN 313337-99-4 CAPLUS
CN 5-Pyrimidinecarboxamide, 2-[[(1R,2R)-2-(dimethylamino)cyclopentyl]amino]-4-[(3-methylphenyl)amino]-6-(phenylmethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



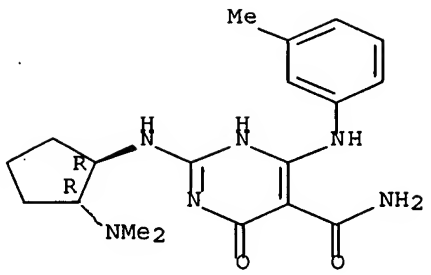
RN 313338-14-6 CAPLUS
CN 5-Pyrimidinecarboxamide, 2-[[(1R,2R)-2-(dimethylamino)cyclohexyl]amino]-1,4-dihydro-6-[(3-methylphenyl)amino]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

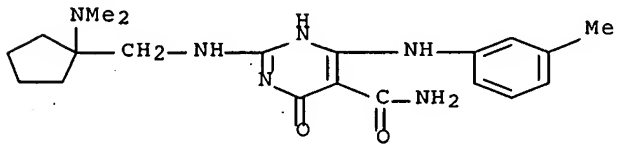


RN 313338-15-7 CAPLUS
CN 5-Pyrimidinecarboxamide, 2-[[(1R,2R)-2-(dimethylamino)cyclopentyl]amino]-1,4-dihydro-6-[(3-methylphenyl)amino]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

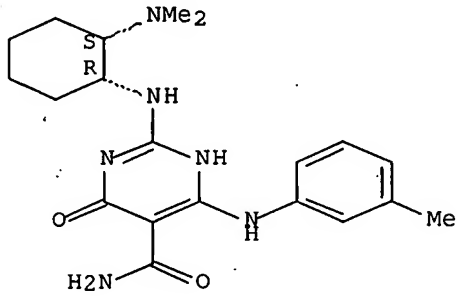


RN 313338-42-0 CAPLUS
CN 5-Pyrimidinecarboxamide, 2-[[[1-(dimethylamino)cyclopentyl]methyl]amino]-1,4-dihydro-6-[(3-methylphenyl)amino]-4-oxo- (9CI) (CA INDEX NAME)



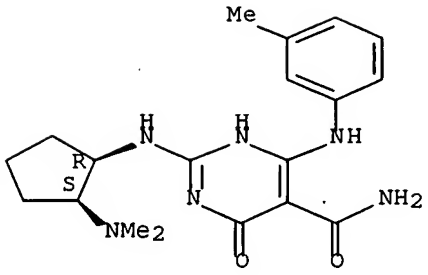
RN 313338-55-5 CAPLUS
CN 5-Pyrimidinecarboxamide, 2-[[(1R,2S)-2-(dimethylamino)cyclohexyl]amino]-1,4-dihydro-6-[(3-methylphenyl)amino]-4-oxo- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 313338-56-6 CAPLUS
CN 5-Pyrimidinecarboxamide, 2-[[(1R,2S)-2-(dimethylamino)cyclopentyl]amino]-1,4-dihydro-6-[(3-methylphenyl)amino]-4-oxo- (9CI) (CA INDEX NAME)

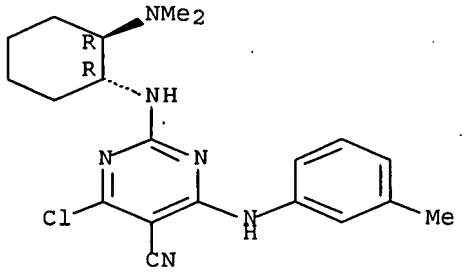
Absolute stereochemistry.



IT 313339-17-2P 313339-18-3P 313339-27-4P
313339-28-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitrogen-containing heterocyclic derivs. as remedies for complications of diabetes)

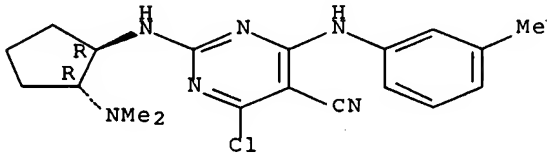
RN 313339-17-2 CAPLUS
CN 5-Pyrimidinecarbonitrile, 4-chloro-2-[[(1R,2R)-2-(dimethylamino)cyclohexyl]amino]-6-[(3-methylphenyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



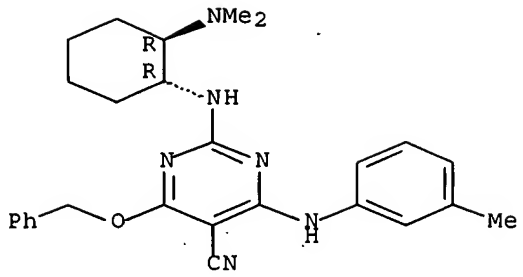
RN 313339-18-3 CAPLUS
CN 5-Pyrimidinecarbonitrile, 4-chloro-2-[[(1R,2R)-2-(dimethylamino)cyclopentyl]amino]-6-[(3-methylphenyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



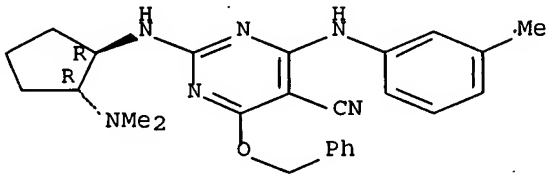
RN 313339-27-4 CAPLUS
CN 5-Pyrimidinecarbonitrile, 2-[[(1R,2R)-2-(dimethylamino)cyclohexyl]amino]-4-[(3-methylphenyl)amino]-6-(phenylmethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 313339-28-5 CAPLUS
CN 5-Pyrimidinecarbonitrile, 2-[[(1R,2R)-2-(dimethylamino)cyclopentyl]amino]-4-[(3-methylphenyl)amino]-6-(phenylmethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



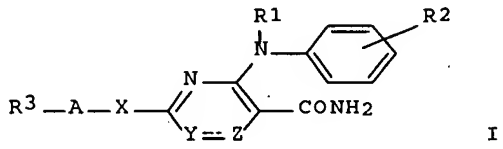
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 21 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:881124 CAPLUS Full-text
DOCUMENT NUMBER: 134:42141
TITLE: Preparation of novel heterocyclic carboxamide derivatives as spleen tyrosine kinase inhibitors
INVENTOR(S): Hisamichi, Hiroyuki; Kawazoe, Souichirou; Tanabe, Kazuhito; Ichikawa, Atsushi; Orita, Akiko; Suzuki, Takayuki; Onda, Kenichi; Takeuchi, Makoto
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000075113	A1	20001214	WO 2000-JP3767	20000609 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
JP 2001055378	A	20010227	JP 2000-171185	20000607 <--

EP 1184376	A1	20020306	EP 2000-935619		20000609 <--
EP 1184376	B1	20050202			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
AT 288420	T	20050215	AT 2000-935619		20000609 <--
PT 1184376	T	20050429	PT 2000-935619		20000609 <--
ES 2237430	T3	20050801	ES 2000-935619		20000609 <--
US 6797706	B1	20040928	US 2001-9276		20011210 <--
PRIORITY APPLN. INFO.:			JP 1999-162692	A	19990609 <--
			WO 2000-JP3767	W	20000609 <--

OTHER SOURCE(S): MARPAT 134:42141
ED Entered STN: 15 Dec 2000
GI



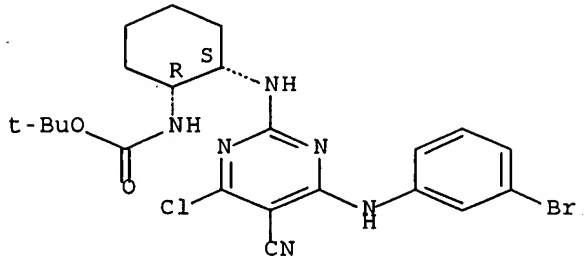
I

AB Nitrogenous six-membered heterocycle compds. bearing as the substituents -X-A-R3, -N-(R1)-(R2-substituted Ph) and -CONH2 [I; wherein A = (substituted) lower alkylene, (substituted) (hetero)arylene, cycloalkylene; X = NR4, CONR4, NR4CO, O, S; the dotted line between Y and Z represents the presence of a bond (Y:Z) or the absence of a bond (Y-Z); Y-Z = NR5-CO, CO-NR5, NR5-NR5, CO-CO; Y:Z = N:CR1, CR7:N, N:N, CR7:CR7; R4 = each H, lower alkyl, -CO-lower alkyl, or -SO2-lower alkyl; R2 = H, (halo-substituted) lower alkyl, -O-lower alkyl, -S-lower alkyl, -O-aryl, nitro, cyano, or the like; R3 = -CO2H, -CO2-lower alkyl, -lower alkylene-CO2H, -NH2, -alkylene-NH2, or the like; R5 = H, lower alkyl; R6 = lower alkyl, OH, -O-lower alkyl, -O-(substituted) aryl, -O-lower alkylene-(substituted) aryl, -NR1-(substituted) aryl, -CO-lower alkyl-(substituted) aryl; R7 = H, R6] salts or prodrugs thereof are prepared Also claimed are spleen tyrosine kinase (Syk) inhibitors containing the compds. I or the salts or the prodrugs thereof as the active ingredient. The compds. I are useful for the prevention or treatment of allergies, inflammations, autoimmune diseases, cancers, transplant rejection, graft-vs.-host diseases, and thrombosis. Thus, 2.76 mL cis-1,2-cyclohexanediamine was added to a mixture of 605 mg 6-chloro-2-(3-methylanilino)pyridine-3-carboxamide and 10 mL MeCN and refluxed for 5 days to give 230 mg 6-(cis-2-aminohexylamino)-2-(3-methylanilino)pyrazine-3-carboxamide (II). II showed IC50 of ≤0.05 μM against Syk, good inhibition against passive cutaneous anaphylaxis (PCA) in mice sensitized by anti-dinitrophenyl-IgE (DNP-IgE), and IC50 of ≤0.1 μM against serotonin release according to the assay described by Collado-Escobar (J. Immunol. 144, 1990).

IT 312736-54-2 312736-56-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of novel heterocyclic carboxamide derivs. as spleen tyrosine kinase inhibitors as preventives or remedies for diseases)

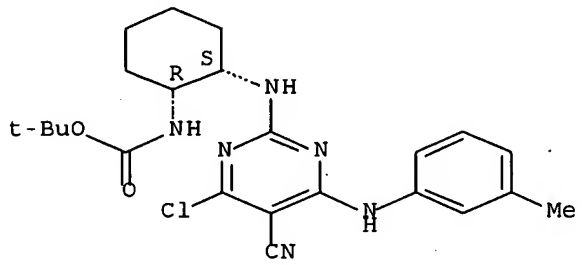
RN 312736-54-2 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[4-[(3-bromophenyl)amino]-6-chloro-5-cyano-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



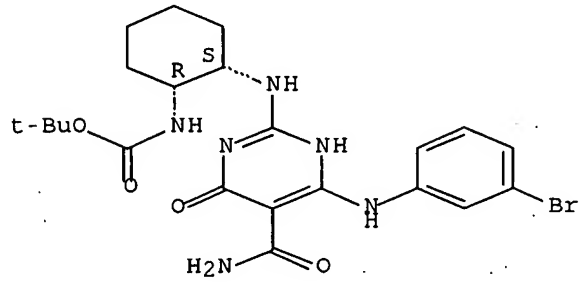
RN 312736-56-4 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[4-chloro-5-cyano-6-[(3-methylphenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



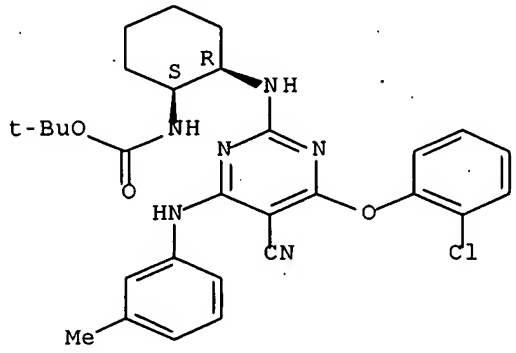
IT 312736-55-3P 312736-63-3P 312736-78-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of novel heterocyclic carboxamide derivs. as spleen tyrosine kinase inhibitors as preventives or remedies for diseases)
RN 312736-55-3 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[5-(aminocarbonyl)-6-[(3-bromophenyl)amino]-1,4-dihydro-4-oxo-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



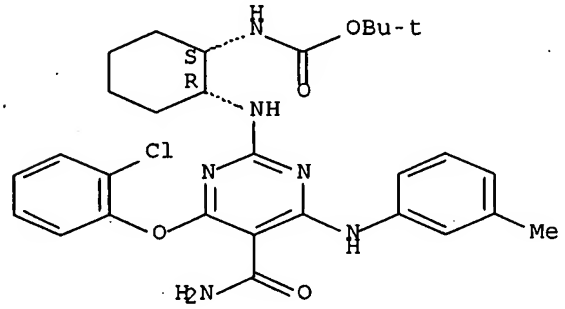
RN 312736-63-3 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[4-(2-chlorophenoxy)-5-cyano-6-[(3-methylphenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 312736-78-0 CAPLUS
CN Carbamic acid, [(1R,2S)-2-[[5-(aminocarbonyl)-4-(2-chlorophenoxy)-6-[(3-methylphenyl)amino]-2-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 22 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:241135 CAPLUS Full-text
DOCUMENT NUMBER: 132:279106
TITLE: Non-peptide GnRH agents, methods and intermediates for their preparation
INVENTOR(S): Anderson, Mark Brian; Vazir, Haresh N.; Luthin, David Robert; Paderes, Genevieve Deguzman; Pathak, Ved P.; Christie, Lance Christopher; Hong, Yufeng; Tompkins, Eileen Valenzuela; Li, Haitao; Faust, James
PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA; et al.
SOURCE: PCT Int. Appl., 444 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 2000020358	A2	20000413	WO 1999-US18790		19990820	<--
WO 2000020358	A3	20001116				
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW						
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG						
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BR 9913374	A	20010515	BR 1999-13374		19990820	<--
EP 1105120	A2	20010613	EP 1999-968010		19990820	<--
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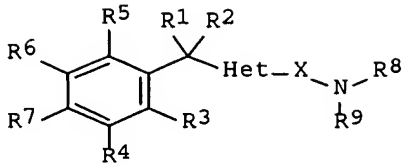
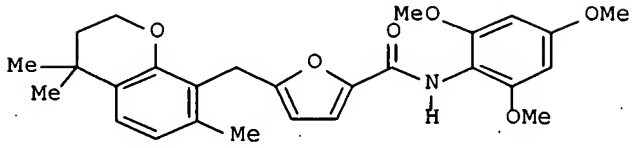
HU 200103622	A2	20020429	HU 2001-3622		19990820	<--
EE 200100102	A	20020617	EE 2001-102		19990820	<--
SI 20746	A	20020630	SI 1999-20076		19990820	<--
TR 200100631	T2	20020821	TR 2001-200100631		19990820	<--
JP 2002535244	T	20021022	JP 2000-574479		19990820	<--
AU 759310	B2	20030410	AU 2000-24709		19990820	<--
NZ 509252	A	20040528	NZ 1999-509252		19990820	<--
AT 291423	T	20050415	AT 1999-968010		19990820	<--
ES 2237966	T3	20050801	ES 1999-968010		19990820	<--
NO 2001000309	A	20010411	NO 2001-309		20010119	<--
IN 2001DN00066	A	20070112	IN 2001-DN66		20010124	<--
ZA 2001000831	A	20020822	ZA 2001-831		20010130	<--
MX 2001PA01834	A	20000821	MX 2001-PA1834		20010219	<--
US 7101878	B1	20060905	US 2001-763216		20010220	<--
LV 12732	B	20020320	LV 2001-45		20010316	<--
BG 105362	A	20011231	BG 2001-105362		20010319	<--
LT 4904	B	20020425	LT 2001-24		20010319	<--
US 2004010033	A1	20040115	US 2003-353160		20030708	<--
PRIORITY APPLN. INFO.:			US 1998-97520P	P	19980820	<--
			WO 1999-US18790	W	19990820	<--
			US 2001-763216	B3	20010220	<--

OTHER SOURCE(S): MARPAT 132:279106
ED Entered STN: 14 Apr 2000
GI



I



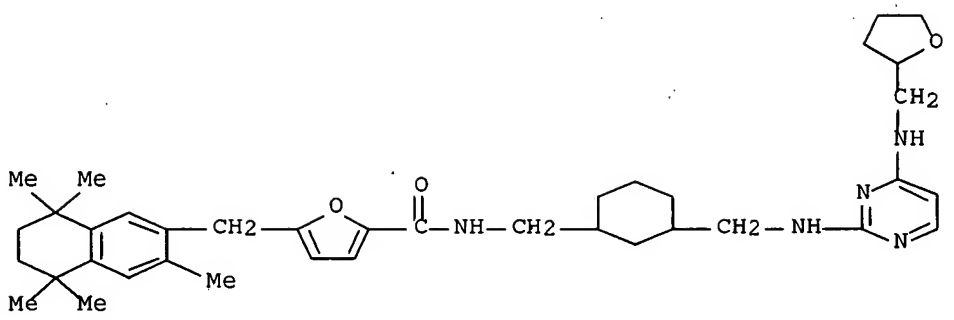
II

AB Non-peptide GnRH agents capable of inhibiting the effect of gonadotropin-releasing hormone are described. The compds. and their pharmaceutically acceptable salts, multimers, prodrugs, and active metabolites are suitable for treating mammalian reproductive disorders and steroid hormone-dependent tumors as well as for regulating fertility, where suppression of gonadotropin release is indicated. The compds. include those of formula I [X = C:O, C:S, S:O, or SO2; Het = 5-membered NOS-heterocycle; R1, R2 = H, alkyl; R3-R7 = H, halo, (un)substituted alkyl, aryl, heteroaryl, CH2OR, OR, CO2R; R = alkyl, aryl, etc.; adjacent rings positions such as R6R7 may form (un)substituted 5- or 6-membered ring with up to 4 heteroatoms; R8 = lipophilic moiety such as alkyl, aryl, CH2OR, OR, etc.; R9 = H, (un)substituted alkyl]. Methods and intermediates for synthesizing the compds. are also described. For instance, 4,4,7-trimethylchroman (preparation given) was alkylated in the 6- and 8-positions using Et 5-(chloromethyl)-2-furoate (46% total yield), and the resulting esters were hydrolyzed to a mixture of acids. This unsepd. mixture was treated with SOCl2 and amidated with 2,4,6-trimethoxyphenylamine- HCl to give the invention compound II and its chroman-6-position isomer, which were separated by HPLC. Several compds. exhibited high affinity (<100 nM) at human GnRH receptors. The compds. antagonized GnRH-stimulated inositol phosphate accumulation in cells with recombinant human GnRH receptors, and an example compound reduced plasma LH levels in castrated male rats. Various biol. data for several hundred compds. are given.

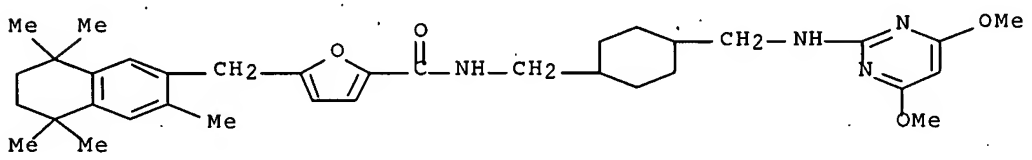
IT 263847-63-8P 263848-23-3P 263848-26-6P
263848-44-8P 263848-45-9P 263848-46-0P
263848-62-0P 263848-88-0P 263849-03-2P
263849-24-7P 263849-27-0P 263851-05-4P
263854-72-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of non-peptide GnRH agents for regulating gonadotropin secretion)

RN 263847-63-8 CAPLUS

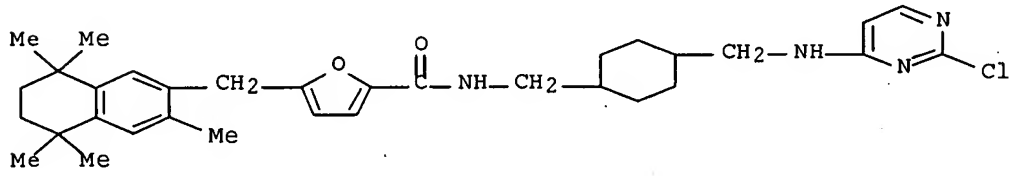
CN 2-Furancarboxamide, N-[[3-[[[4-[[(tetrahydro-2-furanyl)methyl]amino]-2-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



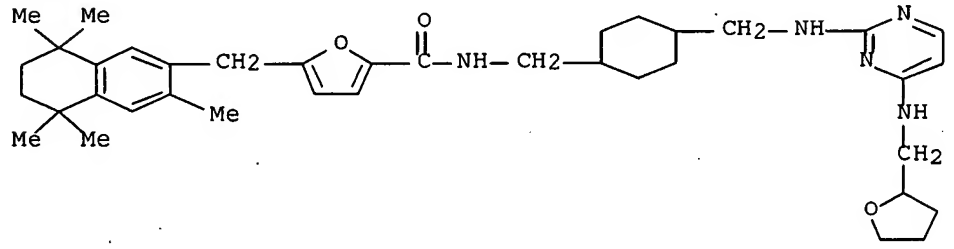
RN 263848-23-3 CAPLUS
CN 2-Furancarboxamide, N-[[4-[[(4,6-dimethoxy-2-pyrimidinyl)amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



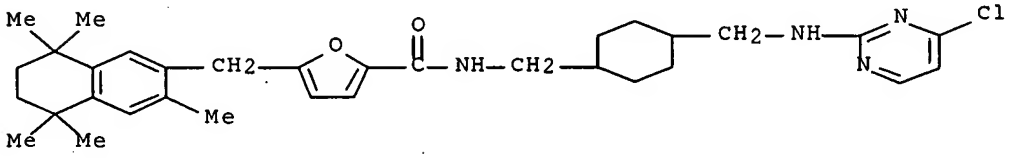
RN 263848-26-6 CAPLUS
CN 2-Furancarboxamide, N-[[4-[[(2-chloro-4-pyrimidinyl)amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



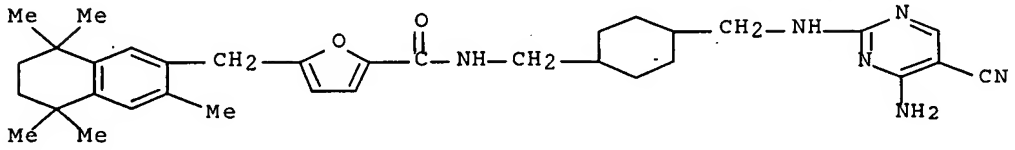
RN 263848-44-8 CAPLUS
CN 2-Furancarboxamide, N-[[4-[[[4-[[(tetrahydro-2-furanyl)methyl]amino]-2-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



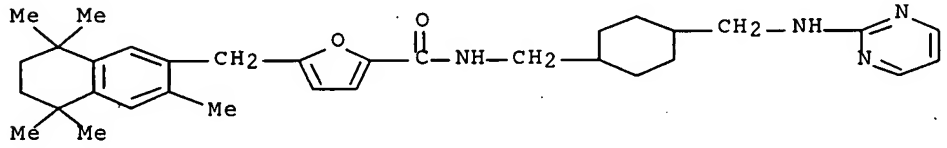
RN 263848-45-9 CAPLUS
CN 2-Furancarboxamide, N-[[4-[[(4-chloro-2-pyrimidinyl)amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



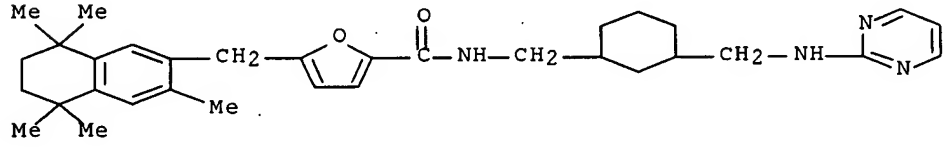
RN 263848-46-0 CAPLUS
CN 2-Furancarboxamide, N-[[4-[[(4-amino-5-cyano-2-pyrimidinyl)amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



RN 263848-62-0 CAPLUS
CN 2-Furancarboxamide, N-[[4-[(2-pyrimidinylamino)methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

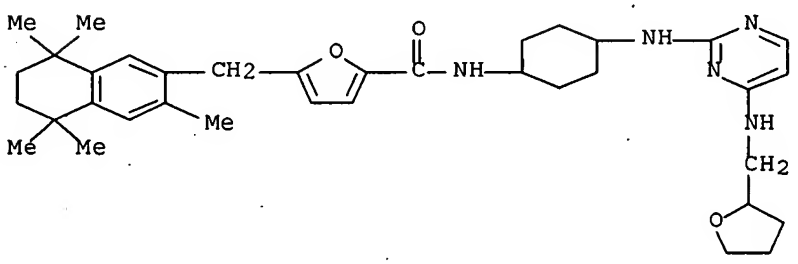


RN 263848-88-0 CAPLUS
CN 2-Furancarboxamide, N-[[3-[(2-pyrimidinylamino)methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



RN 263849-03-2 CAPLUS

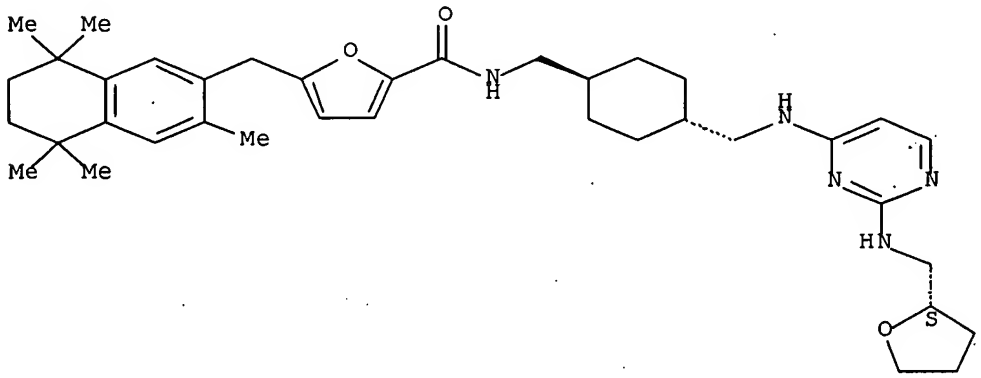
CN 2-Furancarboxamide, N-[4-[[4-[[(tetrahydro-2-furanyl)methyl]amino]-2-pyrimidinyl]amino]cyclohexyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



RN 263849-24-7 CAPLUS

CN 2-Furancarboxamide, N-[[trans-4-[[[2-[[[(2S)-tetrahydro-2-furanyl]methyl]amino]-4-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

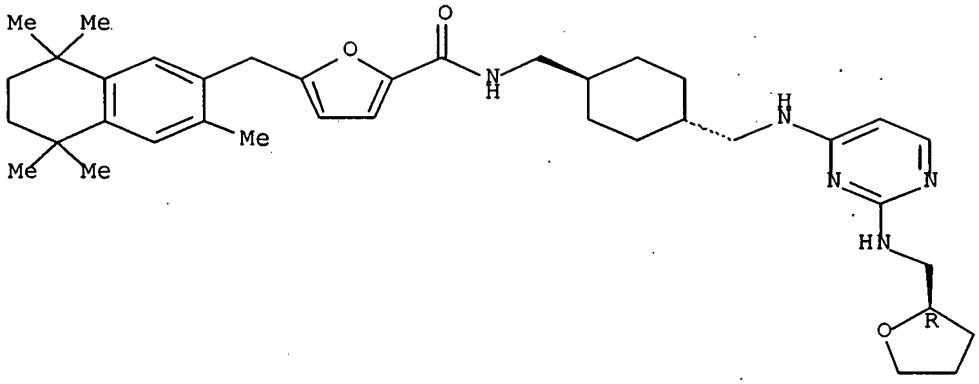
Absolute stereochemistry.



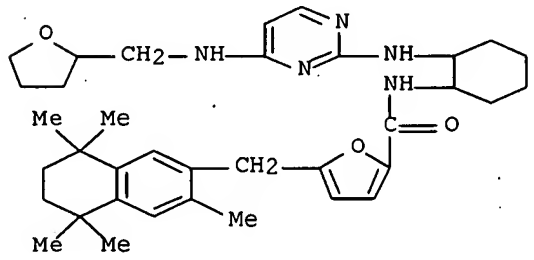
RN 263849-27-0 CAPLUS

CN 2-Furancarboxamide, N-[[trans-4-[[[2-[[[(2R)-tetrahydro-2-furanyl]methyl]amino]-4-pyrimidinyl]amino]methyl]cyclohexyl]methyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)

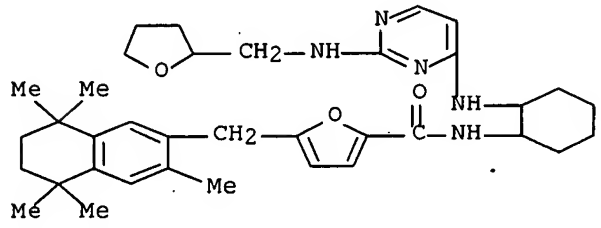
Absolute stereochemistry.



RN 263851-05-4 CAPLUS
CN 2-Furancarboxamide, N-[2-[[4-[[(tetrahydro-2-furanyl)methyl]amino]-2-pyrimidinyl]amino]cyclohexyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



RN 263854-72-4 CAPLUS
CN 2-Furancarboxamide, N-[2-[[2-[[(tetrahydro-2-furanyl)methyl]amino]-4-pyrimidinyl]amino]cyclohexyl]-5-[(5,6,7,8-tetrahydro-3,5,5,8,8-pentamethyl-2-naphthalenyl)methyl]- (9CI) (CA INDEX NAME)



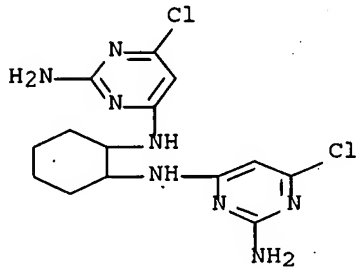
L23 ANSWER 23 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:33829 CAPLUS Full-text
DOCUMENT NUMBER: 132:193982
TITLE: Self-assembly of helical supramolecular channels from chiral aminopyrimidine hydrogen bonding motifs in the solid state
AUTHOR(S): Krische, Michael J.; Lehn, Jean-Marie; Cheung, Eugene;

Vaughn, Gavin; Krische, Amy L.
CORPORATE SOURCE: Laboratoire de chimie supramoleculaire, CNRS ESA 7006, ISIS, CNRS ESA 7006, ISIS, universite Louis-Pasteur, Strasbourg, 67000, Fr.
SOURCE: Comptes Rendus de l'Academie des Sciences, Serie IIc: Chimie (1999), 2(11-13), 549-556
CODEN: CASCFN; ISSN: 1387-1609
PUBLISHER: Editions Scientifiques et Medicales Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 14 Jan 2000
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

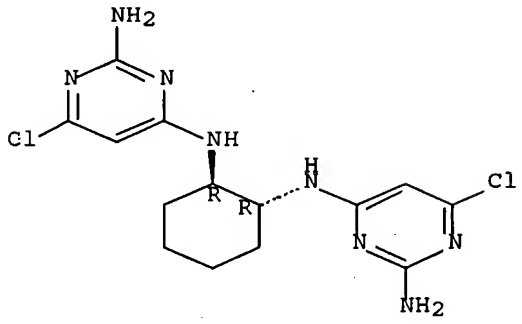
AB The H-bond mediated self-assembly of the chiral C2-sym. bis-(2-amino-4-chloro-pyrimidines) I and II allows for the mol. recognition directed generation of helical superstructures. In the former case, unoccupied channel structures defined by the cylindrical interior of the derived supramol. helix result, as revealed by X-ray crystallog. anal. using a synchrotron source. Upon crystallization, racemic I spontaneously resolves to form homochiral crystals exhibiting a helical packing motif identical to that determined for optically pure I. The data provide insight into the interplay of the different structural and interactional features of the mol. components to the generation of the channel structure and suggest design strategies toward porous organic mol. solids of variable size.

IT 259675-38-2P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(racemate; self-assembly of helical supramol. channels from chiral aminopyrimidine hydrogen bonding motifs in the solid state)
RN 259675-38-2 CAPLUS
CN 2,4-Pyrimidinediamine, N4,N4'-1,2-cyclohexanediylbis[6-chloro- (9CI) (CA INDEX NAME)



IT 259675-37-1P
RL: PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)
(self-assembly of helical supramol. channels from chiral aminopyrimidine hydrogen bonding motifs in the solid state)
RN 259675-37-1 CAPLUS
CN 2,4-Pyrimidinediamine, N4,N4'-(1R,2R)-1,2-cyclohexanediylbis[6-chloro- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

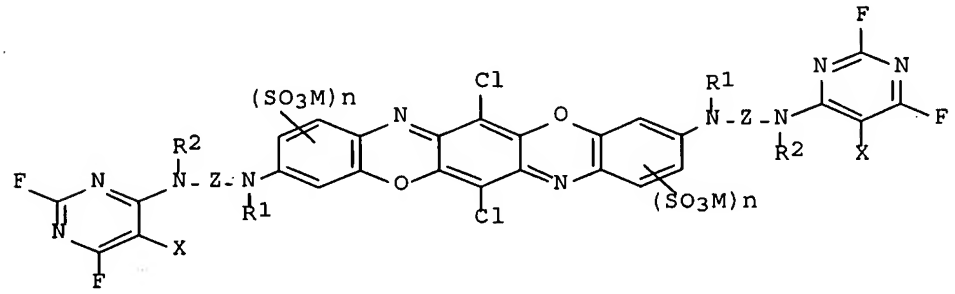


REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 24 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:791797 CAPLUS Full-text
DOCUMENT NUMBER: 132:23860
TITLE: Water-soluble triphenodioxazine reactive dyes, their production and their use
INVENTOR(S): Reiher, Uwe; Brandl, Matthias
PATENT ASSIGNEE(S): DyStar Textilfarben G.m.b.H. und Co. Deutschland K.-G., Germany
SOURCE: Ger. Offen., 10 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19824663	A1	19991209	DE 1998-19824663	19980603 <--
PRIORITY APPLN. INFO.:			DE 1998-19824663	19980603 <--

OTHER SOURCE(S): MARPAT 132:23860
ED Entered STN: 16 Dec 1999
GI



I

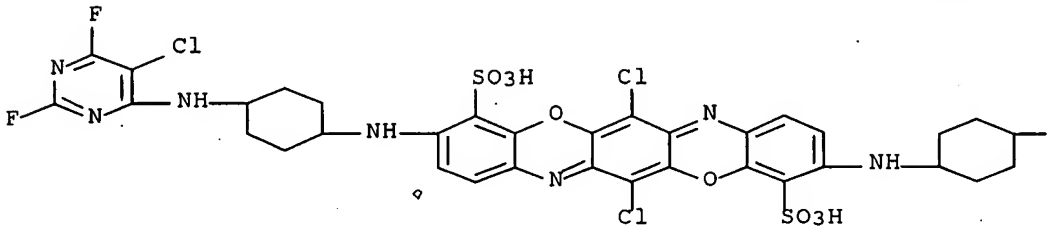
AB The fluoropyrimidine reactive dyes (I; R1, R2 = H, optionally substituted C1-4-alkyl; X = Cl, H; Z = organic connecting group; n = 1, 2) are obtained from triphenodioxazine diamine derivs. and fluoropyrimidines and provide fast blue dyeings on textiles, especially cotton. In an example, I (R1 = R2 = X = H; Z = CH2CH2; n = 1) (λmax 620) is obtained from 2,4,6-trifluoropyrimidine and the appropriate diamine.

IT 252014-68-9P
RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(blue dye; production of water-soluble triphenodioxazine reactive dyes for cotton)

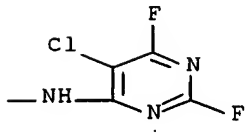
RN 252014-68-9 CAPLUS

CN 4,11-Triphenodioxazinedisulfonic acid, 6,13-dichloro-3,10-bis[[4-[(5-chloro-2,6-difluoro-4-pyrimidinyl)amino]cyclohexyl]amino]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



L23 ANSWER 25 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:404941 CAPLUS Full-text

DOCUMENT NUMBER: 131:44844

TITLE: preparation of novel pyrimidine-5-carboxamide derivatives as tyrosinase inhibitors

INVENTOR(S): Hisamichi, Hiroyuki; Naito, Ryo; Kawazoe, Souichirou; Toyoshima, Akira; Tanabe, Kazuhito; Nakai, Eiichi; Ichikawa, Atsushi; Orita, Akiko; Takeuchi, Makoto

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

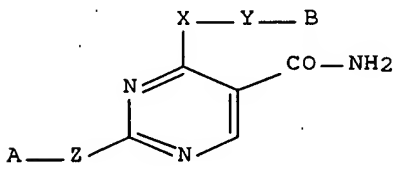
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 9931073 A1 19990624 WO 1998-JP5643 19981214 <--
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SD, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
AU 9915071 A 19990705 AU 1999-15071 19981214 <--
EP 1054004 A1 20001122 EP 1998-959197 19981214 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI
US 6432963 B1 20020813 US 2000-581595 20000615 <--
PRIORITY APPLN. INFO.: JP 1997-344588 A 19971215 <--
WO 1998-JP5643 W 19981214 <--
OTHER SOURCE(S): MARPAT 131:44844
ED Entered STN: 01 Jul 1999
GI



I

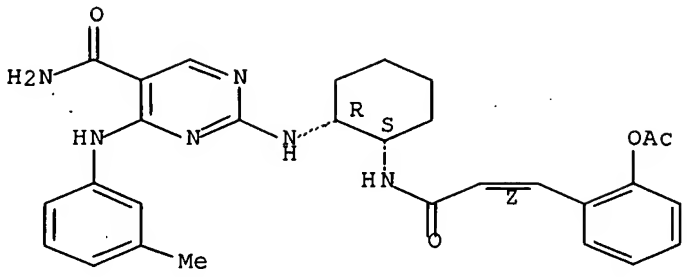
AB Pyrimidine-5-carboxyamide derivs. or salts [I; X = O, S, NR1, CO, NR1CO, CONR1, C=NOR1, a bond; Y = lower alkylene optionally substituted by OR1 or NHR1, a bond; Z = O, NR2, a bond; A = H, optionally substituted lower alkyl, lower alkyl optionally having CO, optionally substituted aryl or heteroaryl, optionally substituted cycloalkyl, optionally substituted and saturated N heterocycle; B = optionally substituted aryl or heteroaryl; R1, R2 = H or lower alkyl optionally containing CO], effective tyrosinase inhibitors useful as 5-HT antagonists, antiallergics, were prepared I showed IC50 < 0.1 μM in scintillation proximity assay. I were effective at 0.1-10 mg/kg-day p.o.

IT 227449-98-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel pyrimidine-5-carboxamide derivs. as tyrosinase inhibitors)

RN 227449-98-1 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[(1R,2S)-2-[[(2Z)-3-[2-(acetyloxy)phenyl]-1-oxo-2-propenyl]amino]cyclohexyl]amino]-4-[(3-methylphenyl)amino]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry as shown.

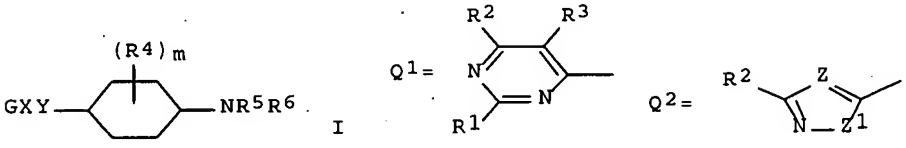


REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 26 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:404940 CAPLUS Full-text
DOCUMENT NUMBER: 131:44606
TITLE: Preparation of cyclohexylamine derivatives as arthropodicides and fungicides
INVENTOR(S): Lee, Kevin Chun
PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA
SOURCE: PCT Int. Appl., 115 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 9931072	A1	19990624	WO 1998-US26013		19981208	<--
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU						
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG						
IN 1997CA01507	A	20050311	IN 1997-CA1507		19970814	<--
AU 9916316	A	19990705	AU 1999-16316		19981208	<--
PRIORITY APPLN. INFO.:			US 1997-69994P	P	19971218	<--
			WO 1998-US26013	W	19981208	<--

OTHER SOURCE(S): MARPAT 131:44606
ED Entered STN: 01 Jul 1999
GI

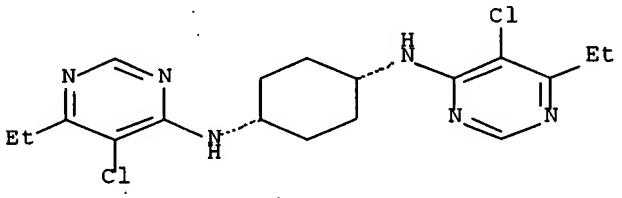


AB The title compds. I [G = Q1, Q2; Y is a direct bond or C1-C4 alkylene optionally substituted with C1-C4 alkyl; X is O, NR7 or S(O)p; each Z is independently selected from N and CR3; each Z1 is independently selected from O, S and NR8; and R1-R8, m and p are as defined in the disclosure], arthropodicides and fungicides, were prepared E.g., cis-N-N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-1,4-cyclohexanediamine was prepared The activity of I against fall armyworm, two-spotted spider mite, Erysiphe graminis, etc., was determined

IT 227469-23-0P 227469-37-6P 227469-68-3P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of cyclohexylamine derivs. as arthropodicides and fungicides)

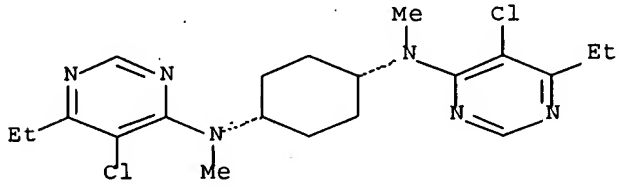
RN 227469-23-0 CAPLUS
CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



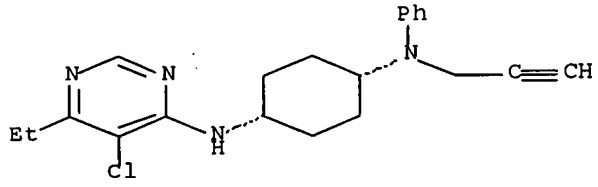
RN 227469-37-6 CAPLUS
CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-N,N'-dimethyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 227469-68-3 CAPLUS
CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-phenyl-N-2-propynyl-, cis- (9CI) (CA INDEX NAME)

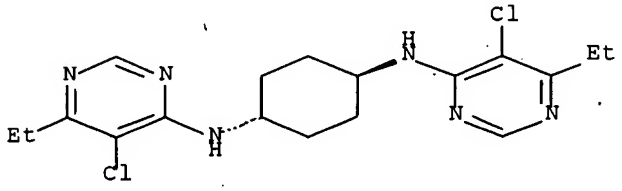
Relative stereochemistry.



IT 227469-24-1P 227469-27-4P 227469-28-5P
227469-30-9P 227469-32-1P 227469-33-2P
227469-34-3P 227469-35-4P 227469-36-5P
227469-38-7P 227469-39-8P 227469-40-1P
227469-41-2P 227469-42-3P 227469-43-4P
227469-44-5P 227469-45-6P 227469-46-7P
227469-47-8P 227469-53-6P 227469-54-7P
227469-55-8P 227469-56-9P 227469-57-0P
227469-58-1P 227469-59-2P 227469-60-5P
227469-61-6P 227469-62-7P 227469-63-8P
227469-64-9P 227469-65-0P 227469-66-1P
227469-67-2P 227469-69-4P 227469-70-7P
227469-71-8P 227469-72-9P 227469-73-0P
227469-74-1P 227469-75-2P 227469-76-3P
227469-77-4P 227469-78-5P 227469-79-6P
227469-80-9P 227469-81-0P 227469-82-1P
227469-83-2P 227469-84-3P 227469-85-4P
227469-86-5P 227469-87-6P 227469-88-7P
227469-89-8P 227469-90-1P 227469-91-2P
227469-92-3P 227469-93-4P 227469-94-5P
227469-95-6P 227470-15-7P 227470-16-8P
227470-17-9P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclohexylamine derivs. as arthropodicides and fungicides)

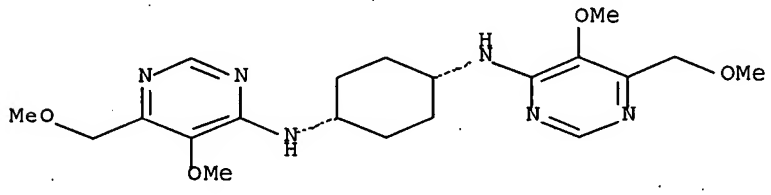
RN 227469-24-1 CAPLUS
CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



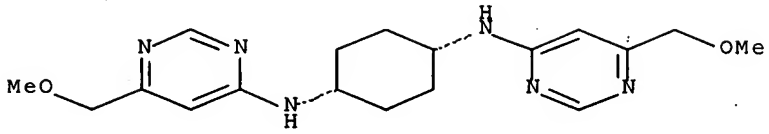
RN 227469-27-4 CAPLUS
CN 1,4-Cyclohexanediamine, N,N'-bis[5-methoxy-6-(methoxymethyl)-4-pyrimidinyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



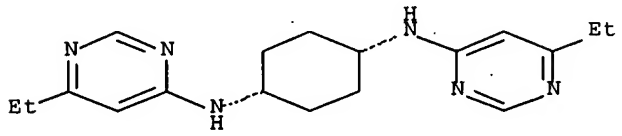
RN 227469-28-5 CAPLUS
CN 1,4-Cyclohexanediamine, N,N'-bis[6-(methoxymethyl)-4-pyrimidinyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



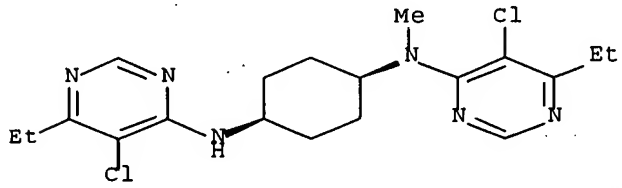
RN 227469-30-9 CAPLUS
CN 1,4-Cyclohexanediamine, N,N'-bis(6-ethyl-4-pyrimidinyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



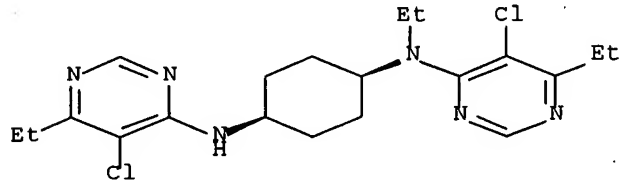
RN 227469-32-1 CAPLUS
CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-N-methyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



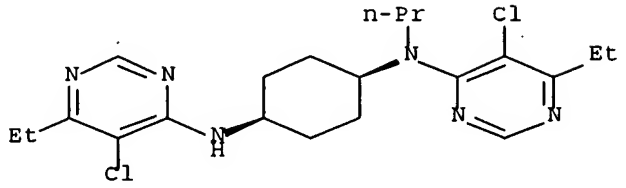
RN 227469-33-2 CAPLUS
CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-N-ethyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



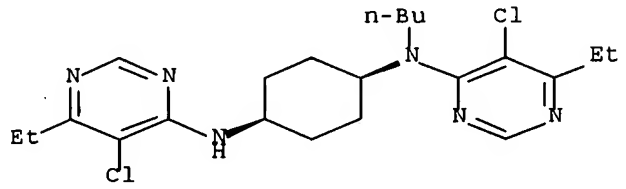
RN 227469-34-3 CAPLUS
CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-N-propyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



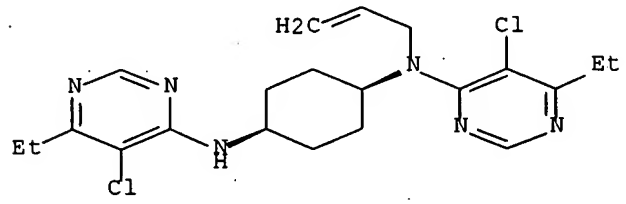
RN 227469-35-4 CAPLUS
CN 1,4-Cyclohexanediamine, N-butyl-N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



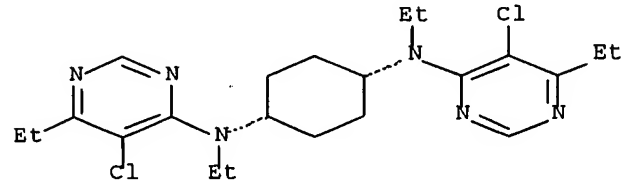
RN 227469-36-5 CAPLUS
CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-N-2-propenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



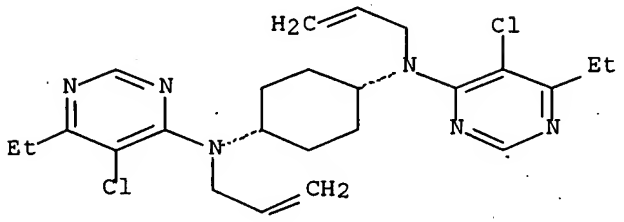
RN 227469-38-7 CAPLUS
CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-N,N'-diethyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



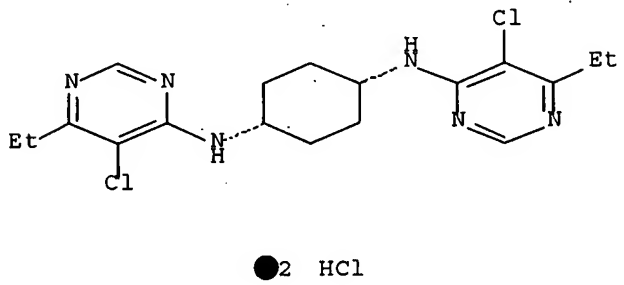
RN 227469-39-8 CAPLUS
CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-N,N'-di-2-propenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 227469-40-1 CAPLUS
CN 1,4-Cyclohexanediamine, N,N'-bis(5-chloro-6-ethyl-4-pyrimidinyl)-, dihydrochloride, cis- (9CI) (CA INDEX NAME)

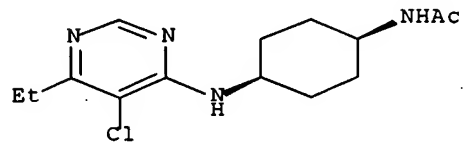
Relative stereochemistry.



●2 HCl

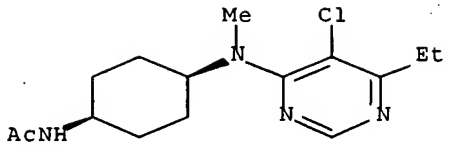
RN 227469-41-2 CAPLUS
CN Acetamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



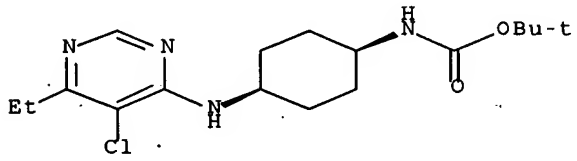
RN 227469-42-3 CAPLUS
CN Acetamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)methylamino]cyclohexyl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



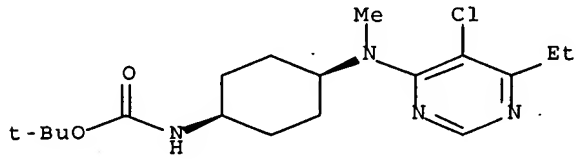
RN 227469-43-4 CAPLUS
CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



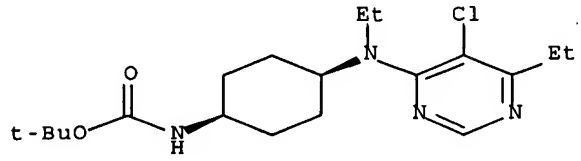
RN 227469-44-5 CAPLUS
CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)methylamino]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



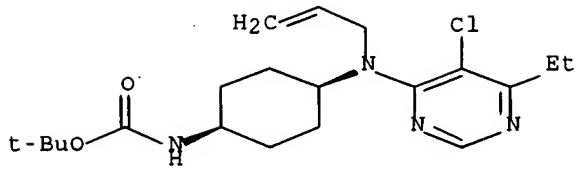
RN 227469-45-6 CAPLUS
CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)ethylamino]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



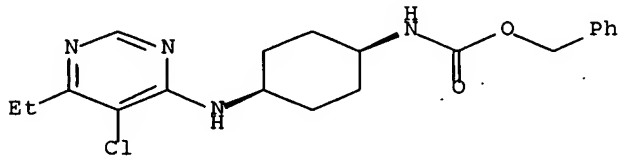
RN 227469-46-7 CAPLUS
CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)-2-propenylamino]cyclohexyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



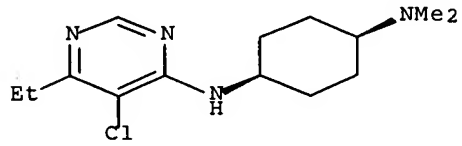
RN 227469-47-8 CAPLUS
CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



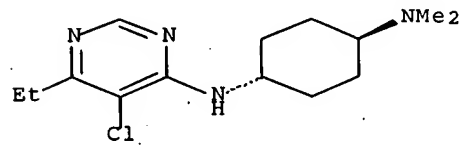
RN 227469-53-6 CAPLUS
CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N,N-dimethyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



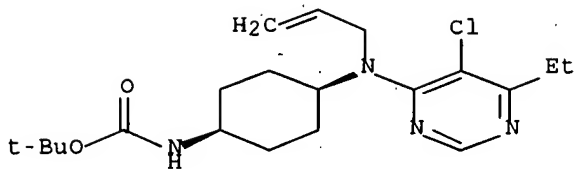
RN 227469-54-7 CAPLUS
CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N,N-dimethyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



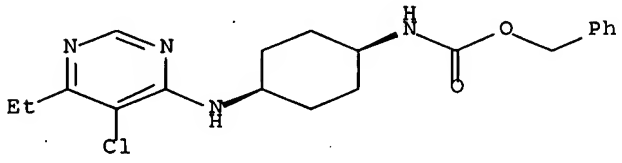
RN 227469-55-8 CAPLUS
CN 1,4-Cyclohexanediamine, N-butyl-N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-methyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



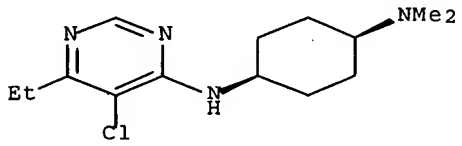
RN 227469-47-8 CAPLUS
CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



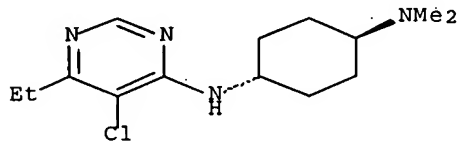
RN 227469-53-6 CAPLUS
CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N,N-dimethyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



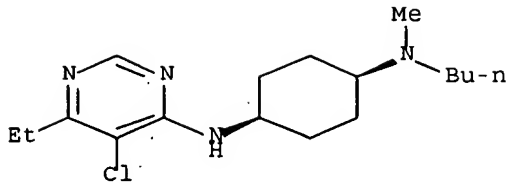
RN 227469-54-7 CAPLUS
CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N,N-dimethyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



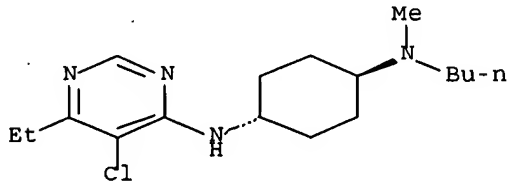
RN 227469-55-8 CAPLUS
CN 1,4-Cyclohexanediamine, N-butyl-N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-methyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



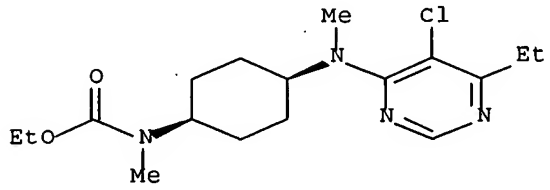
RN 227469-56-9 CAPLUS
CN 1,4-Cyclohexanediamine, N-butyl-N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-methyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



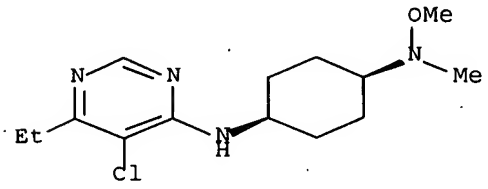
RN 227469-57-0 CAPLUS
CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)methylamino]cyclohexyl]methyl-, ethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



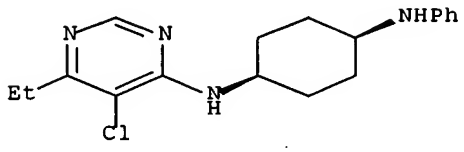
RN 227469-58-1 CAPLUS
CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-methoxy-N-methyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



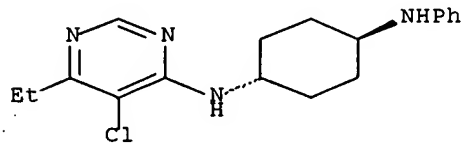
RN 227469-59-2 CAPLUS
CN 1,4-Cyclohexanediamine, N-(5-chloro-6-ethyl-4-pyrimidinyl)-N'-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



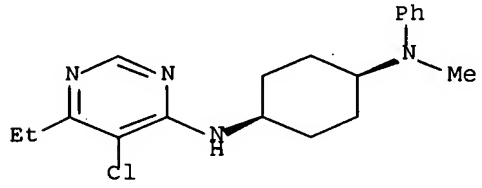
RN 227469-60-5 CAPLUS
CN 1,4-Cyclohexanediamine, N-(5-chloro-6-ethyl-4-pyrimidinyl)-N'-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



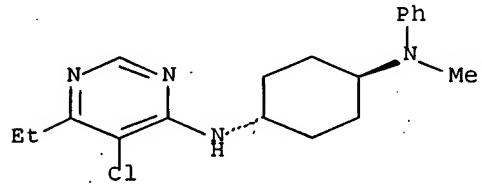
RN 227469-61-6 CAPLUS
CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-methyl-N-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



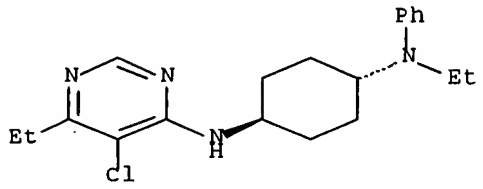
RN 227469-62-7 CAPLUS
CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-methyl-N-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



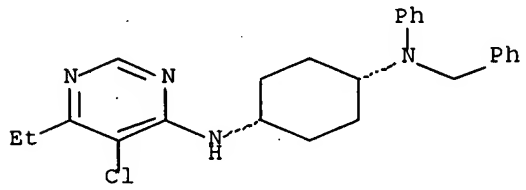
RN 227469-63-8 CAPLUS
CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-ethyl-N-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



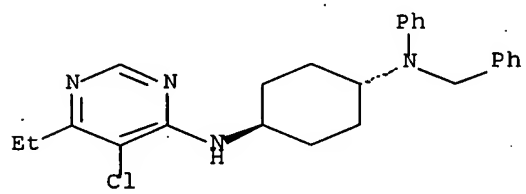
RN 227469-64-9 CAPLUS
CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-phenyl-N-(phenylmethyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



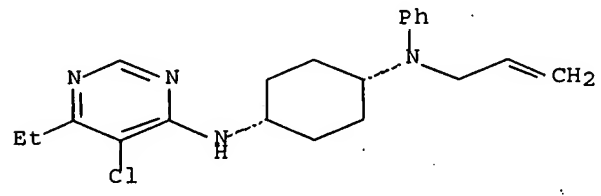
RN 227469-65-0 CAPLUS
CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-phenyl-N-(phenylmethyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 227469-66-1 CAPLUS
CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-phenyl-N-2-propenyl-, cis- (9CI) (CA INDEX NAME)

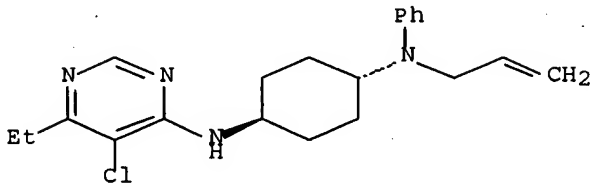
Relative stereochemistry.



RN 227469-67-2 CAPLUS
CN 1,4-Cyclohexanediamine, N'-(5-chloro-6-ethyl-4-pyrimidinyl)-N-phenyl-N-2-

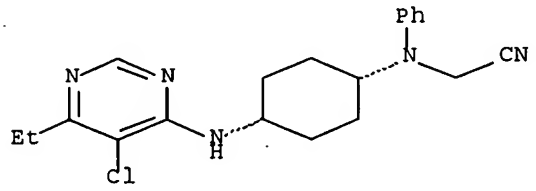
propenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



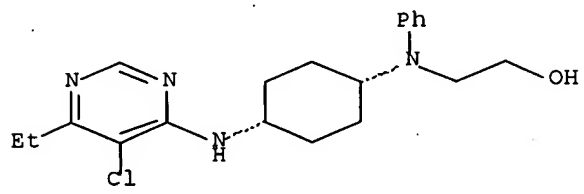
RN 227469-69-4 CAPLUS
CN Acetonitrile, [[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenylamino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



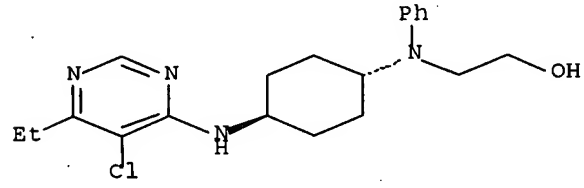
RN 227469-70-7 CAPLUS
CN Ethanol, 2-[[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenylamino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



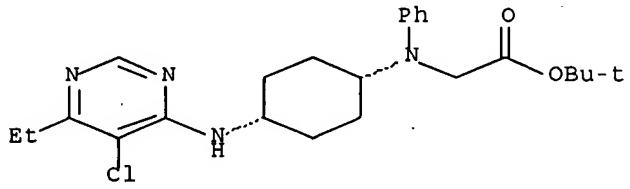
RN 227469-71-8 CAPLUS
CN Ethanol, 2-[[trans-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenylamino]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



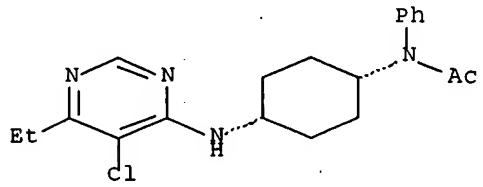
RN 227469-72-9 CAPLUS
CN Glycine, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



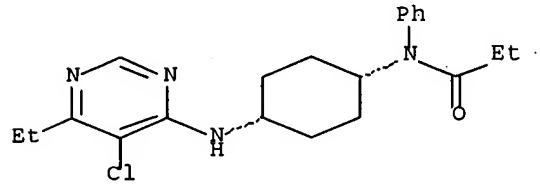
RN 227469-73-0 CAPLUS
CN Acetamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



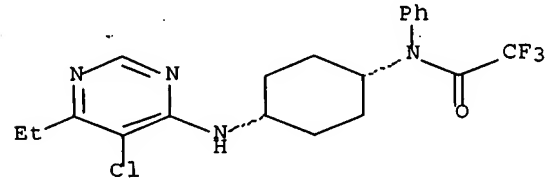
RN 227469-74-1 CAPLUS
CN Propanamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



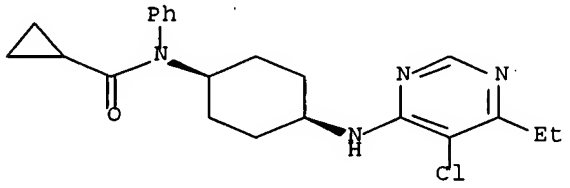
RN 227469-75-2 CAPLUS
CN Acetamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-2,2,2-trifluoro-N-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



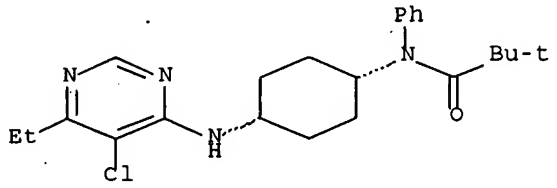
RN 227469-76-3 CAPLUS
CN Cyclopropanecarboxamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



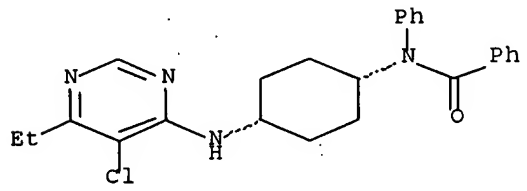
RN 227469-77-4 CAPLUS
CN Propanamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-2,2-dimethyl-N-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



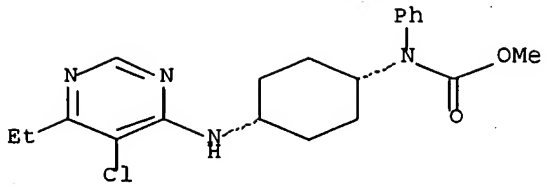
RN 227469-78-5 CAPLUS
CN Benzamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



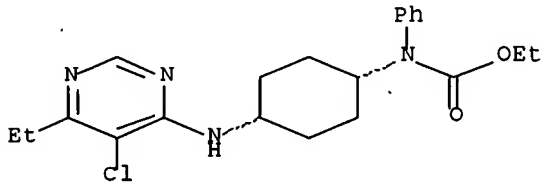
RN 227469-79-6 CAPLUS
CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenyl-, methyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



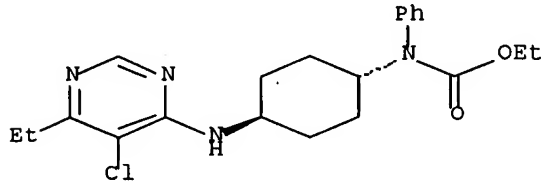
RN 227469-80-9 CAPLUS
CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenyl-, ethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



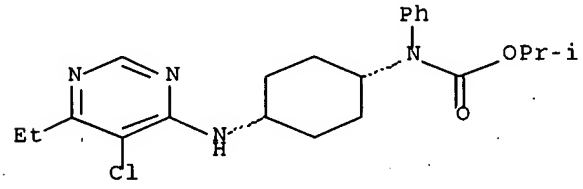
RN 227469-81-0 CAPLUS
CN Carbamic acid, [trans-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenyl-, ethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



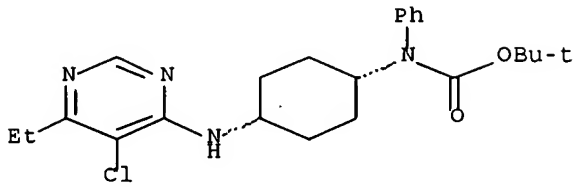
RN 227469-82-1 CAPLUS
CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenyl-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



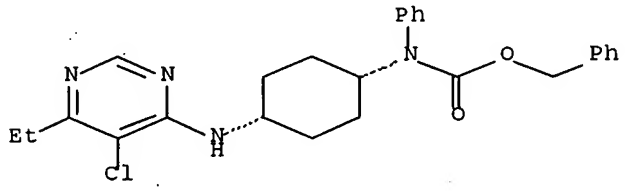
RN 227469-83-2 CAPLUS
CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



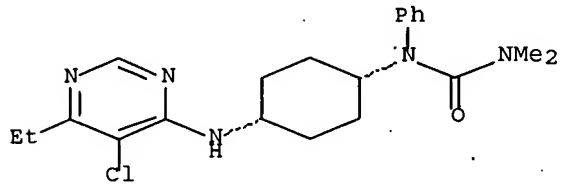
RN 227469-84-3 CAPLUS
CN Carbamic acid, [cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]ph
enyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.



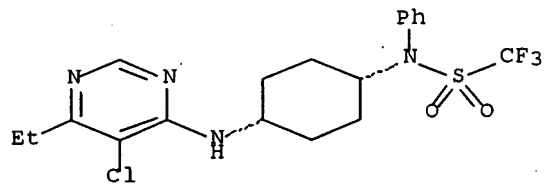
RN 227469-85-4 CAPLUS
CN Urea, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N',N'-
dimethyl-N-phenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 227469-86-5 CAPLUS
CN Methanesulfonamide, N-[cis-4-[(5-chloro-6-ethyl-4-
pyrimidinyl)amino]cyclohexyl]-1,1,1-trifluoro-N-phenyl- (9CI) (CA INDEX
NAME)

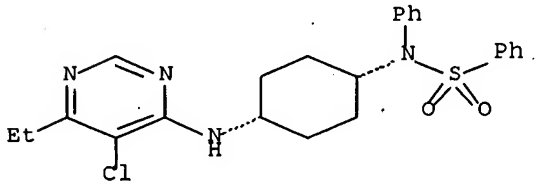
Relative stereochemistry.



RN 227469-87-6 CAPLUS

CN Benzenesulfonamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N-phenyl- (9CI) (CA INDEX NAME)

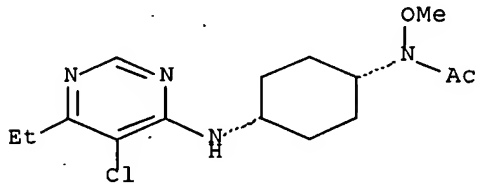
Relative stereochemistry.



RN 227469-88-7 CAPLUS

CN Acetamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N-methoxy- (9CI) (CA INDEX NAME)

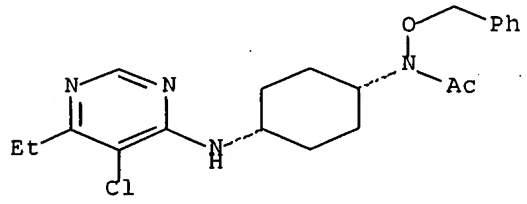
Relative stereochemistry.



RN 227469-89-8 CAPLUS

CN Acetamide, N-[cis-4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]cyclohexyl]-N-(phenylmethoxy)- (9CI) (CA INDEX NAME)

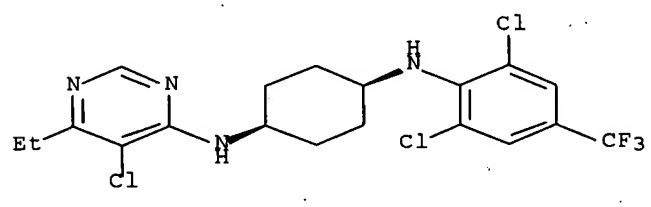
Relative stereochemistry.



RN 227469-90-1 CAPLUS

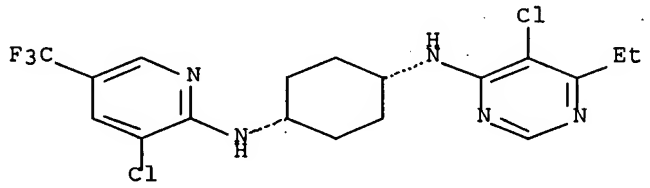
CN 1,4-Cyclohexanediamine, N-(5-chloro-6-ethyl-4-pyrimidinyl)-N'-[2,6-dichloro-4-(trifluoromethyl)phenyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



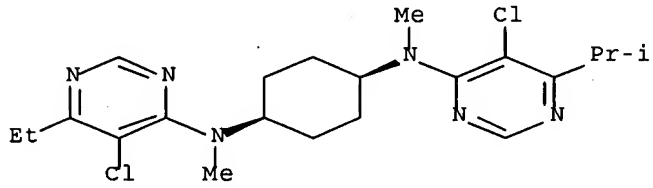
RN 227469-91-2 CAPLUS
CN 1,4-Cyclohexanediamine, N-(5-chloro-6-ethyl-4-pyrimidinyl)-N'-[3-chloro-5-(trifluoromethyl)-2-pyridinyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



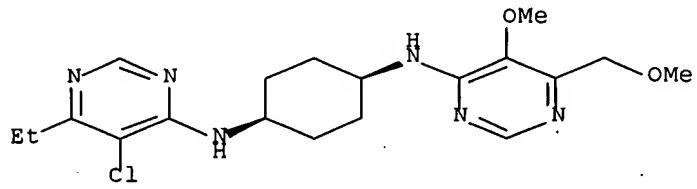
RN 227469-92-3 CAPLUS
CN 1,4-Cyclohexanediamine, N-(5-chloro-6-ethyl-4-pyrimidinyl)-N'-[5-chloro-6-(1-methylethyl)-4-pyrimidinyl]-N,N'-dimethyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



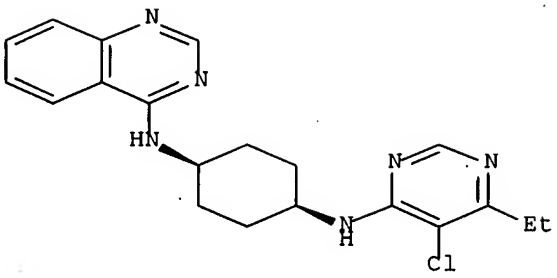
RN 227469-93-4 CAPLUS
CN 1,4-Cyclohexanediamine, N-(5-chloro-6-ethyl-4-pyrimidinyl)-N'-[5-methoxy-6-(methoxymethyl)-4-pyrimidinyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



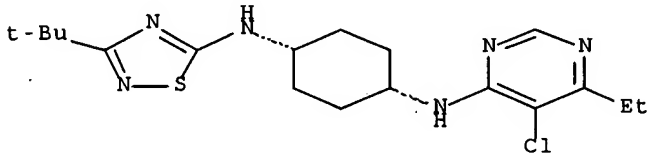
RN 227469-94-5 CAPLUS
CN 1,4-Cyclohexanediamine, N-(5-chloro-6-ethyl-4-pyrimidinyl)-N'-4-quinazolinyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



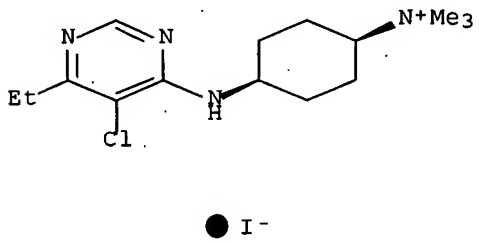
RN 227469-95-6 CAPLUS
CN 1,4-Cyclohexanediamine, N-(5-chloro-6-ethyl-4-pyrimidinyl)-N'-[3-(1,1-dimethylethyl)-1,2,4-thiadiazol-5-yl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



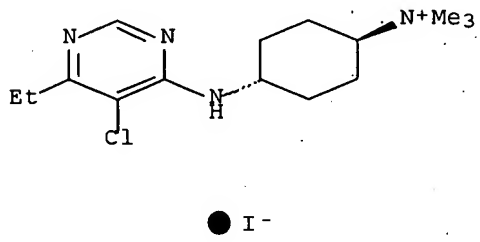
RN 227470-15-7 CAPLUS
CN Cyclohexanaminium, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-N,N,N-trimethyl-, iodide, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



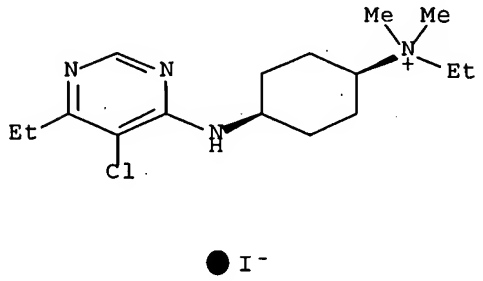
RN 227470-16-8 CAPLUS
CN Cyclohexanaminium, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-N,N,N-trimethyl-, iodide, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 227470-17-9 CAPLUS
CN Cyclohexanaminium, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-N-ethyl-N,N-dimethyl-, iodide, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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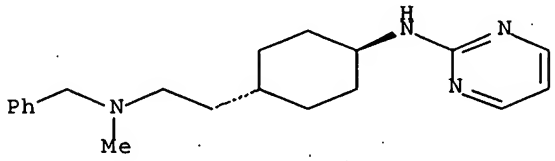
LANGUAGE: English
ED Entered STN: 14 Feb 1998
AB A series of {4-[2-(4-arylpiperazin-1-yl)alkyl]cyclohexyl}pyrimidin-2- ylamines were prepared and found to have receptor binding affinity for D2 and D3 dopamine (DA) receptors and serotonin 5-HT1A receptors. The structural contributions to D2/D3 and 5-HT1A receptor binding of the aminopyrimidine, cycloalkyl, and phenylpiperazine portions of the mol. were examined Compds. having potent affinity for both DA D2 and 5-HT1A receptors were evaluated for intrinsic activity at these receptors, in vitro and in vivo. One of the compds. (PD 158771) had a profile indicative of partial agonist activity at both D2 and 5-HT1A receptors causing partially decreased synthesis of the neurotransmitters DA and 5-HT and their metabolites. This compound has a profile in behavioral tests that is predictive of antipsychotic activity, suggesting that mixed partial agonists may have utility as antipsychotic agents with increased efficacy and decreased side effects.
IT 204245-70-5P 204245-89-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of aminopyrimidines with affinity for serotonin and dopamine receptors)

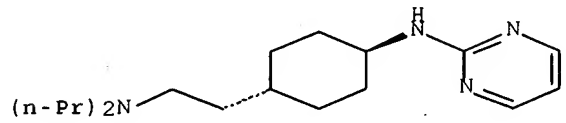
RN 204245-70-5 CAPLUS
CN 2-Pyrimidinamine, N-[4-[2-[methyl(phenylmethyl)amino]ethyl]cyclohexyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 204245-89-6 CAPLUS
CN 2-Pyrimidinamine, N-[4-[2-(dipropylamino)ethyl]cyclohexyl]-, trans- (9CI) (CA INDEX NAME)

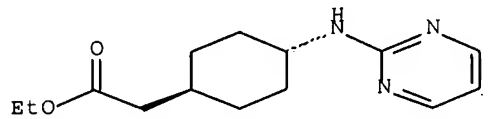
Relative stereochemistry.



IT 189153-07-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of aminopyrimidines with affinity for serotonin and dopamine receptors)

RN 189153-07-9 CAPLUS
CN Cyclohexaneacetic acid, 4-(2-pyrimidinylamino)-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



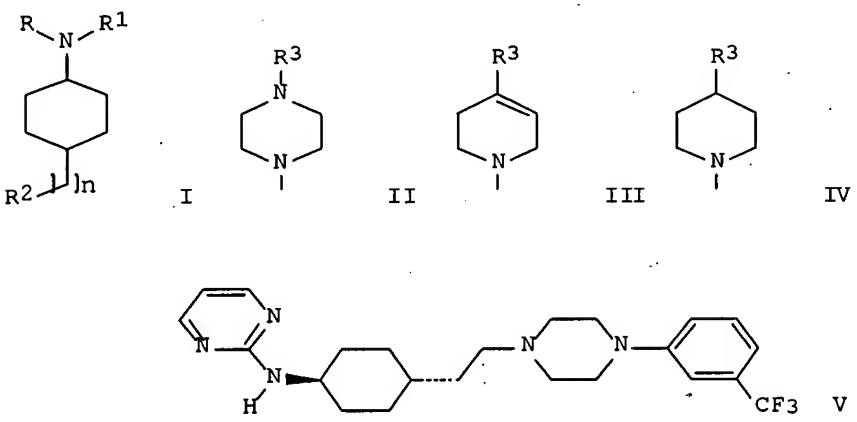
REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 28 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:321401 CAPLUS Full-text
DOCUMENT NUMBER: 126:293365
TITLE: Preparation of heteroaryl-substituted cyclohexylamines as central nervous system (CNS) agents
INVENTOR(S): Belliotti, Thomas R.; Kesten, Suzanne R.; Pugsley,

Thomas A.; Wustrow, David J.
PATENT ASSIGNEE(S): Warner-Lambert Company, USA
SOURCE: PCT Int. Appl., 61 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9711070	A1	19970327	WO 1996-US13687	19960823 <--
W: AU, BG, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KR, LK, LR, LT, LV, MG, MX, NO, NZ, PL, RO, SG, SI, SK, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9668590	A	19970409	AU 1996-68590	19960823 <--
ZA 9607944	A	19970402	ZA 1996-7944	19960919 <--
US 5977110	A	19991102	US 1998-43331	19980320 <--
PRIORITY APPLN. INFO.:			US 1995-4193P P	19950922 <--
			WO 1996-US13687 W	19960823 <--

OTHER SOURCE(S): MARPAT 126:293365
ED Entered STN: 21 May 1997
GI



AB The title compds. [I; R = heteroaryl; R1 = H, lower alkyl, cycloalkyl, aryl, PhCH2; n = 1-2; R2 = II, III, IV (wherein R3 = (un)substituted 2-pyrimidinyl, 2-, 3- or 4-pyridinyl, 2- or 3-thienyl, etc.)], useful as CNS agents, and particularly useful as dopaminergic, serotonergic, antipsychotic, and anxiolytic agents, and for treatment of schizophrenia, were prepared Thus, reaction of trans-(4-aminocyclohexyl)acetic acid Et ester with 2-chloropyrimidine in the presence of Et3N in EtOH followed by reduction of the resulting trans-[4-(pyrimidin-2-ylamino)cyclohexyl]acetic acid Et ester with LiAlH4 in THF, treatment of trans-[4-(pyrimidin-2- ylamino)cyclohexyl]ethanol with CBr4 in the presence of polymer-supported Ph3P in CH2Cl2, and reaction of trans-[4-(2-bromoethyl)cyclohexyl]pyrimidi n-2-ylamine with 1-(3-

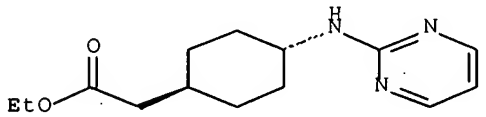
trifluoromethylphenyl)piperazine in the presence of K2CO3 in MeCN afforded trans-V which showed Ki of 6 nM against [3H]N-0437 binding to h-D2 receptors.

IT 189153-07-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heteroaryl-substituted cyclohexylamines as central nervous system (CNS) agents)

RN 189153-07-9 CAPLUS

CN Cyclohexaneacetic acid, 4-(2-pyrimidinylamino)-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L23 ANSWER 29 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:391643 CAPLUS Full-text

DOCUMENT NUMBER: 125:58537

TITLE: Preparation of 4-cyclohexylaminopyrimidine derivatives for agrohorticultural pest control

INVENTOR(S): Obata, Tokio; Fujii, Katsutoshi; Tsutsumiuchi, Kiyoshi; Yamanaka, Yoshinori

PATENT ASSIGNEE(S): Japan

SOURCE: PCT Int. Appl., 83 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

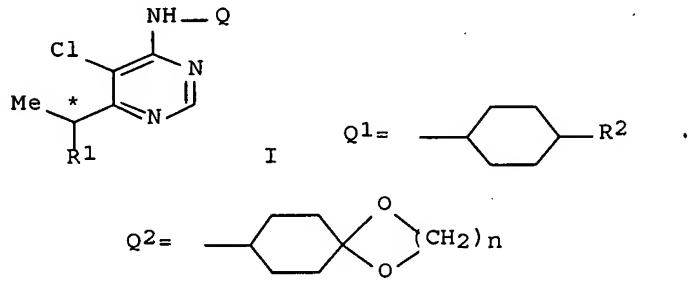
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9606086	A1	19960229	WO 1995-JP1665	19950823 <--
W: KR, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 08113564	A	19960507	JP 1995-213416	19950822 <--
JP 3211636	B2	20010925		
PRIORITY APPLN. INFO.:			JP 1994-198262 A	19940823 <--

OTHER SOURCE(S): MARPAT 125:58537

ED Entered STN: 09 Jul 1996

GI

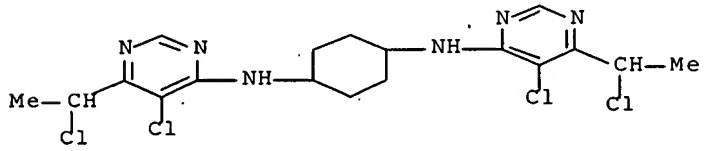


AB The title compds. (I; R1 = halo, C2-5 acyloxy, hydroxy, C1-4 alkoxy, C1-4 alkylthio; Q = Q1, Q2; wherein R2 = C1-8 alkyl, Ph, pyrimidinylamino, C1-6 alkoxy, CO2R3, amino, NHCOR4; wherein R3 = C1-4 alkyl, H; R4 = C1-8 alkyl or alkoxy; the asterisked C atom represents an asym. C atom), useful as insecticides, acaricides, and fungicides, are prepared Thus, a mixture of cis- and trans-4-tert-butylcyclohexylamine (3 g) was dissolved in PhMe, treated with 6.3 g 4,5-dichloro-6-(1-chloroethyl)pyrimidine, and heated with stirring at .apprx.60° for 4 h to give 1.3 g cis-I (R1 = Cl, Q = Q1, R2 = tert-butyl) (II) and 0.9 g trans-I (R1 = Cl, Q = Q1, R2 = tert-butyl). Rice seedlings, which were dipped in a 300 ppm solution of the cis-isomer II and dried, killed 100% Nephotettix cincticeps larvae.

IT 178202-34-1P 178202-35-2P 178202-36-3P
178202-37-4P 178202-38-5P 178202-39-6P
178202-40-9P 178202-61-4P 178202-62-5P
178202-63-6P 178202-64-7P 178202-65-8P
178202-67-0P 178202-68-1P 178202-69-2P
178202-70-5P 178202-71-6P 178202-72-7P
178202-73-8P 178202-74-9P 178202-75-0P
178202-76-1P 178202-77-2P 178202-78-3P
178203-12-8P 178203-13-9P 178203-14-0P
178203-15-1P 178203-16-2P 178203-18-4P
178203-19-5P 178203-20-8P 178203-21-9P
178203-22-0P 178203-23-1P 178203-24-2P
178203-25-3P 178203-26-4P 178203-27-5P
178203-28-6P 178203-29-7P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of (cyclohexylamino)pyrimidine derivs. for agrohorticultural pest control)

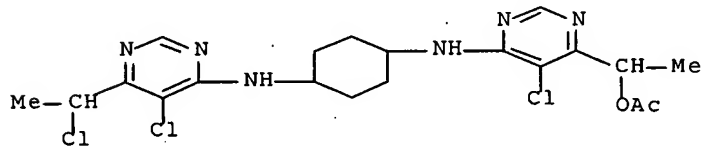
RN 178202-34-1 CAPLUS

CN 1,4-Cyclohexanediamine, N,N'-bis[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

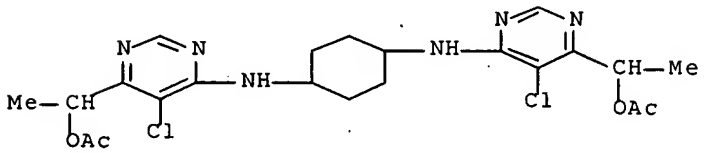


RN 178202-35-2 CAPLUS

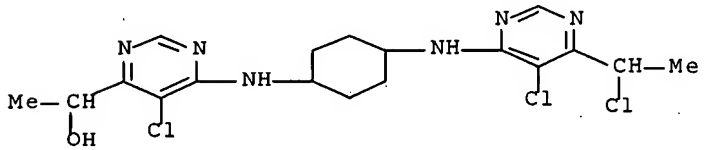
CN 4-Pyrimidinemethanol, 5-chloro-6-[[4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]cyclohexyl]amino]-α-methyl-, acetate (ester) (9CI) (CA INDEX NAME)



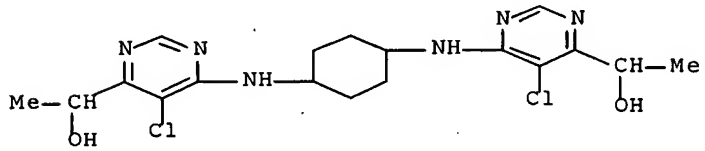
RN 178202-36-3 CAPLUS
CN 4-Pyrimidinemethanol, 5,5'-(1,4-cyclohexanediyldiimino)bis[5-chloro-α-methyl-, diacetate (ester) (9CI) (CA INDEX NAME)



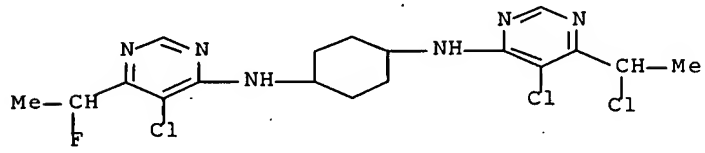
RN 178202-37-4 CAPLUS
CN 4-Pyrimidinemethanol, 5-chloro-6-[[4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]cyclohexyl]amino]-α-methyl- (9CI) (CA INDEX NAME)



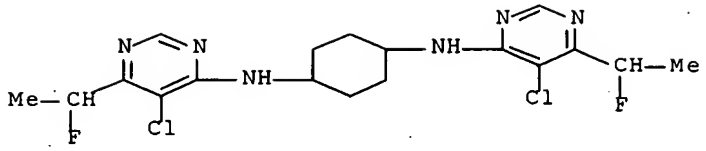
RN 178202-38-5 CAPLUS
CN 4-Pyrimidinemethanol, 5,5'-(1,4-cyclohexanediyldiimino)bis[5-chloro-α-methyl- (9CI) (CA INDEX NAME)



RN 178202-39-6 CAPLUS
CN 1,4-Cyclohexanediamine, N-[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]-N'-[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

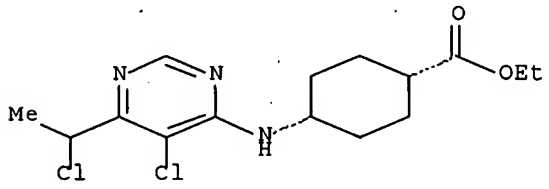


RN 178202-40-9 CAPLUS
CN 1,4-Cyclohexanediamine, N,N'-bis[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



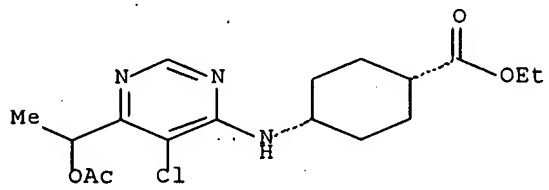
RN 178202-61-4 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



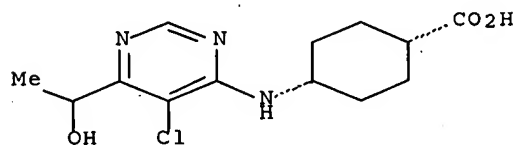
RN 178202-62-5 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[6-[1-(acetyloxy)ethyl]-5-chloro-4-pyrimidinyl]amino]-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



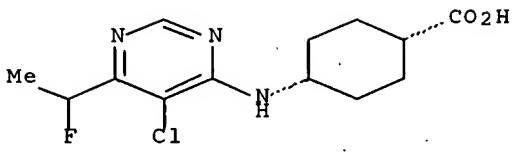
RN 178202-63-6 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[5-chloro-6-(1-hydroxyethyl)-4-pyrimidinyl]amino]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



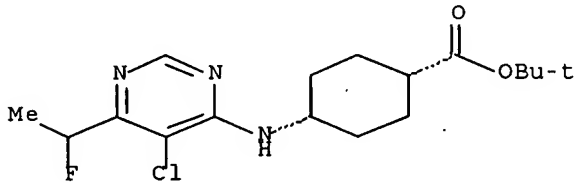
RN 178202-64-7 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



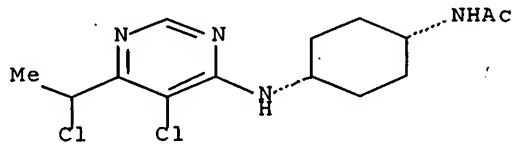
RN 178202-65-8 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]-, 1,1-dimethylethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



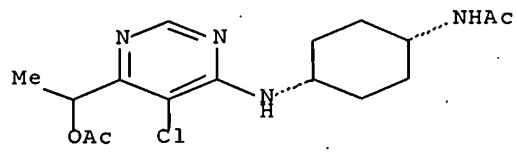
RN 178202-67-0 CAPLUS
CN Acetamide, N-[4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]cyclohexyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



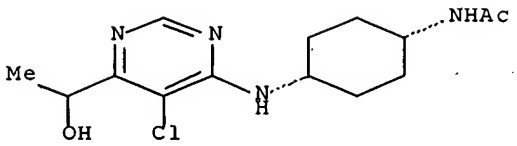
RN 178202-68-1 CAPLUS
CN Acetamide, N-[4-[[6-[1-(acetyloxy)ethyl]-5-chloro-4-pyrimidinyl]amino]cyclohexyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



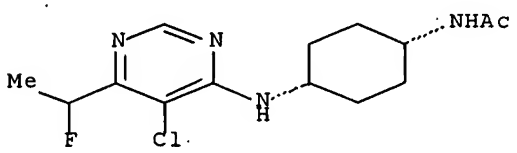
RN 178202-69-2 CAPLUS
CN Acetamide, N-[4-[[5-chloro-6-(1-hydroxyethyl)-4-pyrimidinyl]amino]cyclohexyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



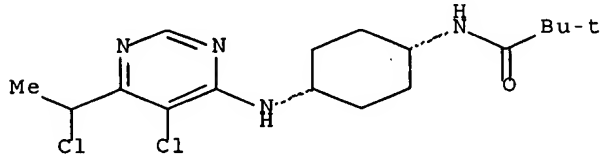
RN 178202-70-5 CAPLUS
CN Acetamide, N-[4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]cyclohexyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



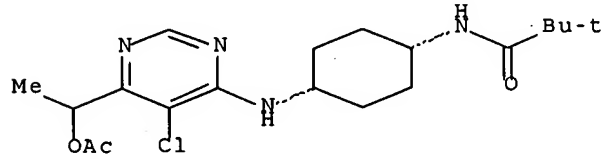
RN 178202-71-6 CAPLUS
CN Propanamide, N-[4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]cyclohexyl]-2,2-dimethyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



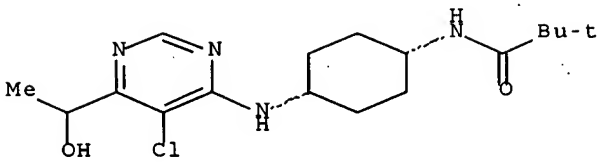
RN 178202-72-7 CAPLUS
CN Propanamide, N-[4-[[6-[1-(acetyloxy)ethyl]-5-chloro-4-pyrimidinyl]amino]cyclohexyl]-2,2-dimethyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



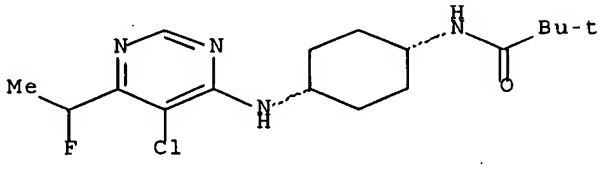
RN 178202-73-8 CAPLUS
CN Propanamide, N-[4-[[5-chloro-6-(1-hydroxyethyl)-4-pyrimidinyl]amino]cyclohexyl]-2,2-dimethyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



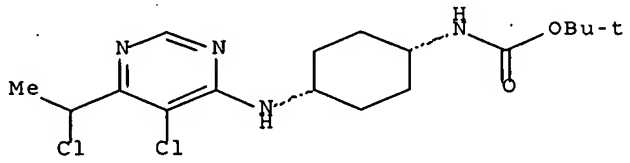
RN 178202-74-9 CAPLUS
CN Propanamide, N-[4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]cyclohexyl]-2,2-dimethyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



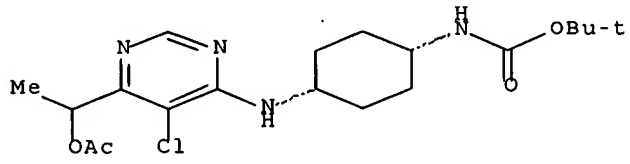
RN 178202-75-0 CAPLUS
CN Carbamic acid, [4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



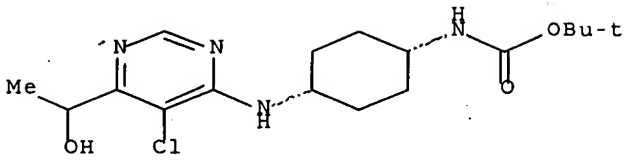
RN 178202-76-1 CAPLUS
CN Carbamic acid, [4-[[6-[1-(acetyloxy)ethyl]-5-chloro-4-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



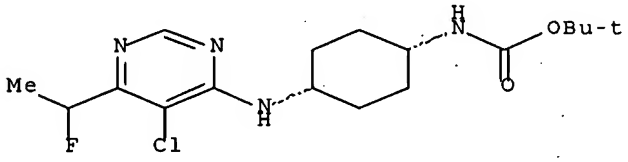
RN 178202-77-2 CAPLUS
CN Carbamic acid, [4-[[5-chloro-6-(1-hydroxyethyl)-4-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



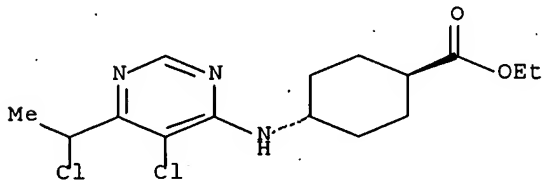
RN 178202-78-3 CAPLUS
CN Carbamic acid, [4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



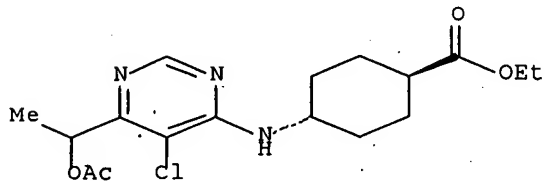
RN 178203-12-8 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



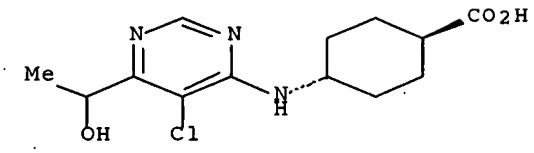
RN 178203-13-9 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[6-[1-(acetyloxy)ethyl]-5-chloro-4-pyrimidinyl]amino]-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



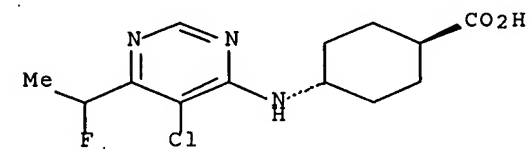
RN 178203-14-0 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[5-chloro-6-(1-hydroxyethyl)-4-pyrimidinyl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



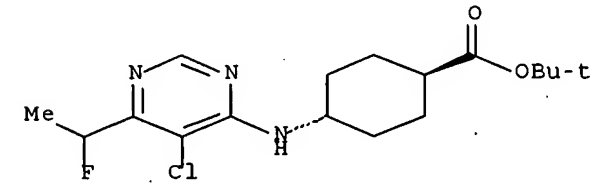
RN 178203-15-1 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



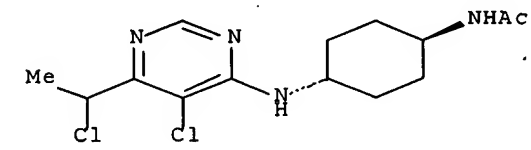
RN 178203-16-2 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



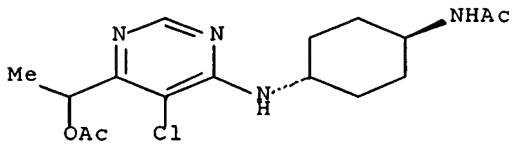
RN 178203-18-4 CAPLUS
CN Acetamide, N-[4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]cyclohexyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



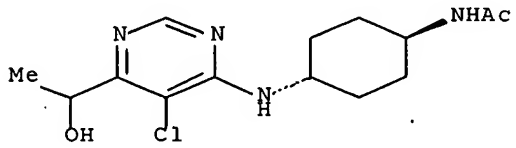
RN 178203-19-5 CAPLUS
CN Acetamide, N-[4-[[6-[1-(acetyloxy)ethyl]-5-chloro-4-pyrimidinyl]amino]cyclohexyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



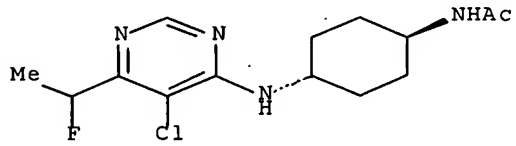
RN 178203-20-8 CAPLUS
CN Acetamide, N-[4-[[5-chloro-6-(1-hydroxyethyl)-4-pyrimidinyl]amino]cyclohexyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



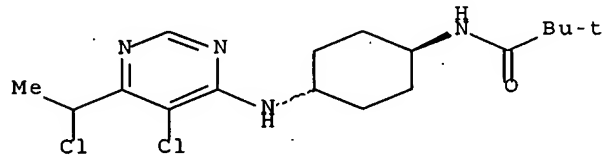
RN 178203-21-9 CAPLUS
CN Acetamide, N-[4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]cyclohexyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



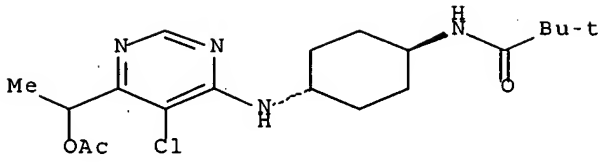
RN 178203-22-0 CAPLUS
CN Propanamide, N-[4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]cyclohexyl]-2,2-dimethyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



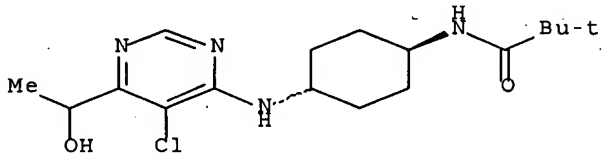
RN 178203-23-1 CAPLUS
CN Propanamide, N-[4-[[6-[1-(acetyloxy)ethyl]-5-chloro-4-pyrimidinyl]amino]cyclohexyl]-2,2-dimethyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



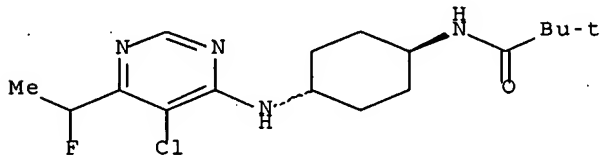
RN 178203-24-2 CAPLUS
CN Propanamide, N-[4-[[5-chloro-6-(1-hydroxyethyl)-4-pyrimidinyl]amino]cyclohexyl]-2,2-dimethyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



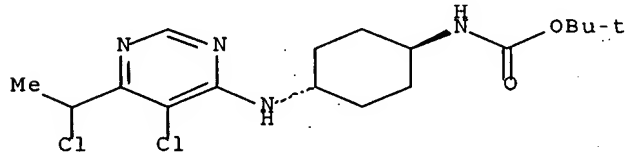
RN 178203-25-3 CAPLUS
CN Propanamide, N-[4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]cyclohexyl]-2,2-dimethyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



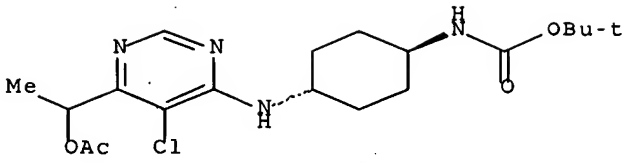
RN 178203-26-4 CAPLUS
CN Carbamic acid, [4-[[5-chloro-6-(1-chloroethyl)-4-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



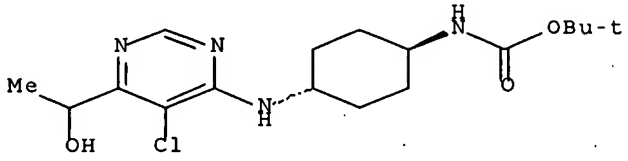
RN 178203-27-5 CAPLUS
CN Carbamic acid, [4-[[6-[1-(acetyloxy)ethyl]-5-chloro-4-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



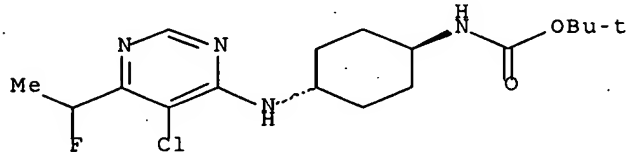
RN 178203-28-6 CAPLUS
CN Carbamic acid, [4-[[5-chloro-6-(1-hydroxyethyl)-4-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 178203-29-7 CAPLUS
CN Carbamic acid, [4-[[5-chloro-6-(1-fluoroethyl)-4-pyrimidinyl]amino]cyclohexyl]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

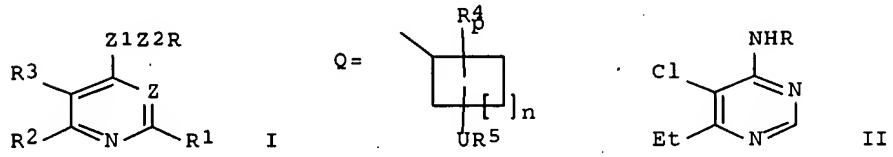


L23 ANSWER 30 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:369682 CAPLUS Full-text
DOCUMENT NUMBER: 125:33666
TITLE: Preparation of 4-(cycloalkylamino)pyrimidines and analogs as pesticides and agrochemical fungicides
INVENTOR(S): Maerkl, Martin; Schaper, Wokfgang; Knauf, Werner; Sanft, Ulrich; Kern, Manfred; Bonin, Werner; Linkies, Adolf Heinz; Reuschling, Dieter Bernd
PATENT ASSIGNEE(S): Hoechst Schering AgrEvo GmbH, Germany
SOURCE: Ger. Offen., 23 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4437137	A1	19960425	DE 1994-4437137	19941018 <--
CA 2202987	A1	19960425	CA 1995-2202987	19951005 <--

WO 9611913		A1	19960425	WO 1995-EP3928	19951005 <--
W:	AL, AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, UZ, VN				
RW:	KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9537454		A	19960506	AU 1995-37454	19951005 <--
EP 787128		A1	19970806	EP 1995-935432	19951005 <--
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, NL, PT, SE				
CN 1161034		A	19971001	CN 1995-195734	19951005 <--
BR 9509378		A	19971014	BR 1995-9378	19951005 <--
HU 77374		A2	19980330	HU 1997-2046	19951005 <--
JP 10507188		T	19980714	JP 1995-512899	19951005 <--
IN 1995MA01304		A	20050225	IN 1995-MA1304	19951010 <--
US 5889012		A	19990330	US 1995-543794	19951016 <--
ZA 9508749		A	19960513	ZA 1995-8749	19951017 <--
PRIORITY APPLN. INFO.:				DE 1994-4437137 A	19941018 <--
				WO 1995-EP3928 W	19951005 <--

OTHER SOURCE(S): CASREACT 125:33666; MARPAT 125:33666
ED Entered STN: 27 Jun 1996
GI



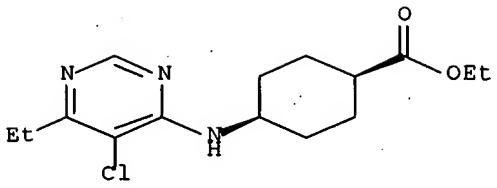
AB Title compds. [I; R = cycloalkyl group Q; R1 = H, (halo)(cyclo)alkyl; R2,R3 = H, halo, alkyl, alkoxy, etc.; R2R3 = atoms to form a ring; R4 = H, halo, (halo)alkyl, alkoxy, alkylthio; R5 = alk(en)yl, aryl, heterocyclyl, etc.; U = bond, O, SO0-2; Z = CH or N; Z1 = NH, O, SO0-2; Z2 = bond, alkylene; n = 0-4; p = 1 or 2] were prepared Thus, 4,5-dichloro-6- ethylpyrimidine was aminated by 4-isopropenylcyclohexylamine (predominantly cis)(preparation given) to give title compound II (R = cis-4-isopropenylcyclohexyl) which gave complete kill of Nilaparvata lugens on rice seedlings at 250ppm.

IT 173843-97-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 4-(cycloalkylamino)pyrimidines and analogs as pesticides and
agrochem. fungicides)

RN 173843-97-5 CAPLUS

CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, ethyl ester, cis- (9CI) (CA INDEX NAME)

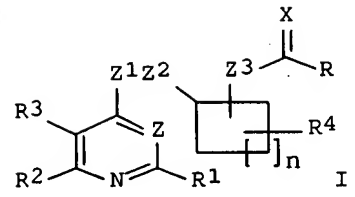
Relative stereochemistry.



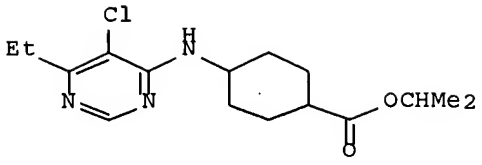
L23 ANSWER 31 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:127981 CAPLUS Full-text
DOCUMENT NUMBER: 124:176139
TITLE: Preparation of pyrimidinylimino- and -oxycycloalkanecarboxylates and analogs as agrochemical fungicides and pesticides
INVENTOR(S): Schaper, Wolfgang; Preus, Rainer; Braun, Peter; Knauf, Werner; Sachse, Burkhard; Waltersdorfer, Anna; Kern, Manfred; Luemmen, Peter; Bonin, Werner
PATENT ASSIGNEE(S): Hoechst Schering AgrEvo GmbH, Germany
SOURCE: Ger. Offen., 56 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4417163	A1	19951123	DE 1994-4417163	19940517 <--
CA 2190495	A1	19951123	CA 1995-2190495	19950503 <--
WO 9531441	A1	19951123	WO 1995-EP1666	19950503 <--
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TT, UA, UZ, VN				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9525235	A	19951205	AU 1995-25235	19950503 <--
AU 703538	B2	19990325		
EP 759909	A1	19970305	EP 1995-919376	19950503 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, NL, PT, SE				
CN 1148383	A	19970423	CN 1995-193115	19950503 <--
BR 9507647	A	19970909	BR 1995-7647	19950503 <--
HU 76722	A2	19971028	HU 1996-3196	19950503 <--
JP 10500115	T	19980106	JP 1995-529316	19950503 <--
US 5691321	A	19971125	US 1995-441217	19950515 <--
ZA 9503957	A	19960119	ZA 1995-3957	19950516 <--
PRIORITY APPLN. INFO.:			DE 1994-4417163 A	19940517 <--
			WO 1995-EP1666 W	19950503 <--

OTHER SOURCE(S): MARPAT 124:176139
ED Entered STN: 02 Mar 1996
GI



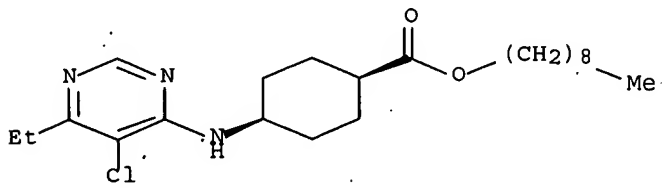
I



II

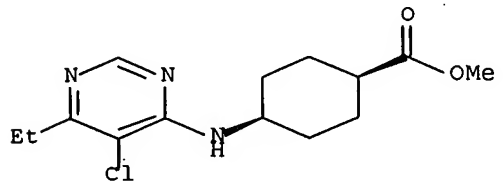
AB Title compds. [I; R = H, OH, alkyl, alkoxy, (di)(alkyl)amino, etc.; R1 = H, halo, (cyclo)alkyl; R2 = H, halo, (cyclo)alkyl, alkoxy, etc.; R3 = H, halo, (halo)alkyl, (halo)alkoxy, etc.; R2R3 = atoms to form a ring; R4 = H, alkyl; X = O or S; Z = CH or N; Z1 = O, S, NH; Z2 = bond, alkylene; Z3 = O, bond; n = 0-5] were prepared Thus, 4,5-dichloro-6-ethylpyrimidine was aminated by Me cis-4-aminocyclohexanecarboxylate to give, after transesterification, title compound II which gave complete control of Nilaparvata lugens on rice seedlings at 250ppm.

IT 173843-88-4P 173843-89-5P 173843-90-8P
173843-91-9P 173843-92-0P 173843-97-5P
173843-98-6P 173843-99-7P 173844-00-3P
173844-01-4P 173844-02-5P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinylimino- and -oxycycloalkanecarboxylates and analogs as agrochem. fungicides and pesticides)
stereochemistry.



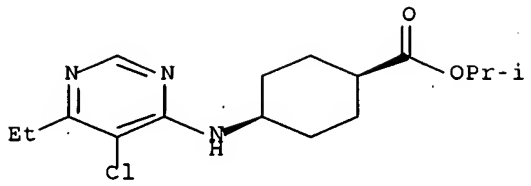
RN 173843-88-4 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



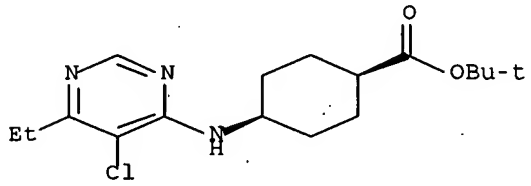
RN 173843-89-5 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, 1-methylethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



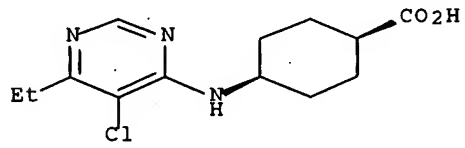
RN 173843-90-8 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, 1,1-dimethylethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



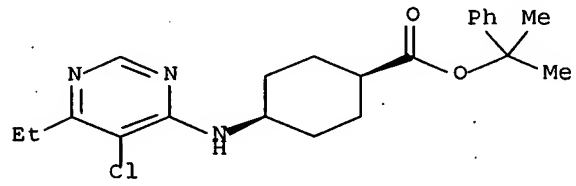
RN 173843-91-9 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



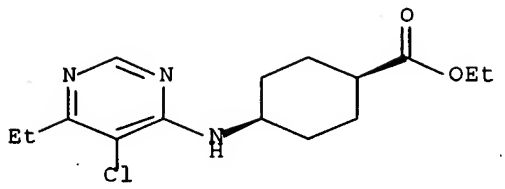
RN 173843-92-0 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, 1-methyl-1-phenylethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



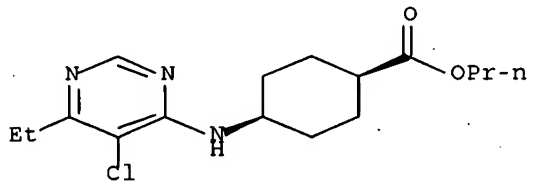
RN 173843-97-5 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



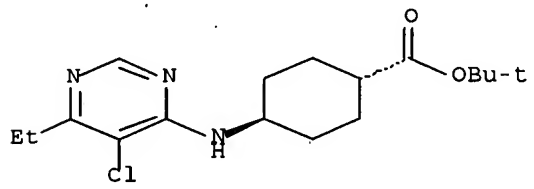
RN 173843-98-6 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, propyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



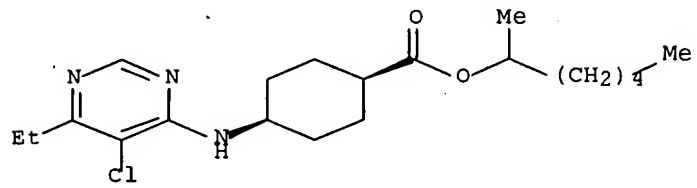
RN 173843-99-7 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, 1,1-dimethylethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 173844-00-3 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, 1-methylhexyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

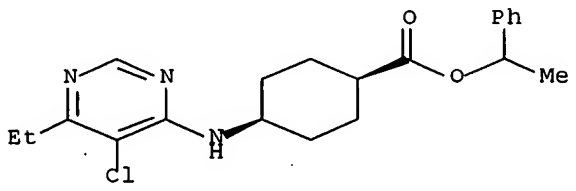


RN 173844-01-4 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, nonyl ester, cis- (9CI) (CA INDEX NAME)

Relative

RN 173844-02-5 CAPLUS
CN Cyclohexanecarboxylic acid, 4-[(5-chloro-6-ethyl-4-pyrimidinyl)amino]-, 1-phenylethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

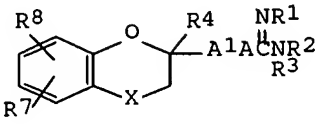


L23 ANSWER 32 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:508815 CAPLUS Full-text
DOCUMENT NUMBER: 121:108815
TITLE: [(Benzodioxane, benzofuran or benzopyran)alkylamino]alkyl-substituted guanidine selective vasoconstrictors
INVENTOR(S): Van Lommen, Guy Rosalia Eugene; De Bruyn, Marcel Frans Leopold; Janssens, Walter Jacobus Joseph
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

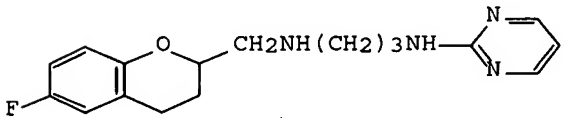
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9317017	A1	19930902	WO 1993-EP435	19930219 <--
W: AU, BB, BG, BR, CA, CZ, FI, HU, JP, KP, KR, LK, MG, MN, MW, NO, NZ, PL, PT, RO, RU, SD, SK, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9334991	A	19930913	AU 1993-34991	19930219 <--
AU 664237	B2	19951109		
EP 639192	A1	19950222	EP 1993-904017	19930219 <--
EP 639192	B1	19960515		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 07504408	T	19950518	JP 1993-514541	19930219 <--
JP 2779268	B2	19980723		
HU 71129	A2	19951128	HU 1994-2464	19930219 <--
HU 222495	B1	20030728		
AT 138064	T	19960615	AT 1993-904017	19930219 <--
ES 2087721	T3	19960716	ES 1993-904017	19930219 <--
CZ 282092	B6	19970514	CZ 1994-2020	19930219 <--
PL 174736	B1	19980930	PL 1993-304902	19930219 <--
RU 2121999	C1	19981120	RU 1994-41210	19930219 <--
SK 280166	B6	19990910	SK 1994-1029	19930219 <--
RO 115630	B1	20000428	RO 1994-1432	19930219 <--
CA 2117483	C	20010109	CA 1993-2117483	19930219 <--

CN 1079470	A	19931215	CN 1993-103671		19930226 <--
CN 1038032	B	19980415			
ZA 9301404	A	19940826	ZA 1993-1404		19930226 <--
LT 3049	B	19941025	LT 1993-367		19930226 <--
LV 10715	B	19951220	LV 1993-149		19930226 <--
IL 104868	A	19980104	IL 1993-104868		19930226 <--
US 5541180	A	19960730	US 1994-256995		19940729 <--
FI 9403928	A	19940826	FI 1994-3928		19940826 <--
FI 109122	B1	20020531			
NO 9403186	A	19940829	NO 1994-3186		19940829 <--
NO 306255	B1	19991011			
US 5607949	A	19970304	US 1996-632227		19960415 <--
US 5624952	A	19970429	US 1996-632226		19960415 <--
US 5688952	A	19971118	US 1996-632228		19960415 <--
US 5703115	A	19971230	US 1996-632230		19960415 <--
PRIORITY APPLN. INFO.:			US 1992-842560	A2	19920227 <--
			WO 1993-EP435	A	19930219 <--
			US 1994-256995	A3	19940729 <--

OTHER SOURCE(S): CASREACT 121:108815; MARPAT 121:108815
ED Entered STN: 03 Sep 1994
GI



I



@ 2HCl

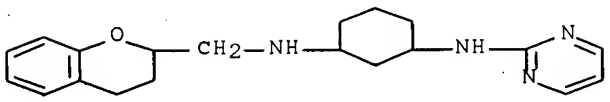
II

AB The title compds. [I; A = bivalent radical; A1 = bivalent C1-3 alkanediyl radical; R1, R3, R4 = H, C1-6 alkyl; R2 = H, C1-6 alkyl, C3-6 alkenyl, C3-6 alkynyl; R7, R8 = H, halogen, C1-6 alkyl, OH, C3-6 alkenyl, C3-6 alkynyl, CN, CO2H, (un)substituted NH2; X = O, CH2, direct bond], which have selective vasoconstrictor activity, are prepared and I-containing formulations presented. Thus, dihydrochloride salt II was prepared (m.p. 139.9°) and demonstrated 50% of the constrictive response obtained with serotonin upon pig basilar arteries at 1.46 + 10-7 M concentration

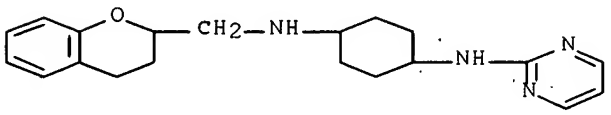
IT 155429-41-7P 155429-48-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and selective vasoconstrictor activity of)

RN 155429-41-7 CAPLUS

CN 1,3-Cyclohexanediamine, N-[(3,4-dihydro-2H-1-benzopyran-2-yl)methyl]-N'-2-pyrimidinyl- (9CI) (CA INDEX NAME)

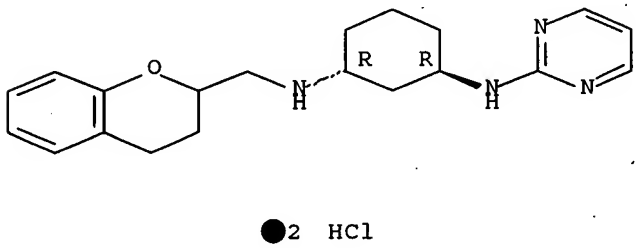


RN 155429-48-4 CAPLUS
CN 1,4-Cyclohexanediamine, N-[(3,4-dihydro-2H-1-benzopyran-2-yl)methyl]-N'-2-pyrimidinyl- (9CI) (CA INDEX NAME)



IT 155426-33-8P 155426-34-9P 155426-39-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 155426-33-8 CAPLUS
CN 1,3-Cyclohexanediamine, N-[(3,4-dihydro-2H-1-benzopyran-2-yl)methyl]-N'-2-pyrimidinyl-, dihydrochloride, trans- (9CI) (CA INDEX NAME)

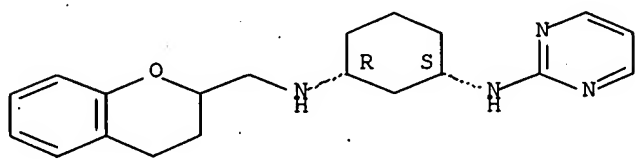
Relative stereochemistry.



●2 HCl

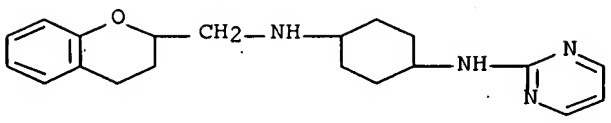
RN 155426-34-9 CAPLUS
CN 1,3-Cyclohexanediamine, N-[(3,4-dihydro-2H-1-benzopyran-2-yl)methyl]-N'-2-pyrimidinyl-, dihydrochloride, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



●2 HCl

RN 155426-39-4 CAPLUS
CN 1,4-Cyclohexanediamine, N-[(3,4-dihydro-2H-1-benzopyran-2-yl)methyl]-N'-2-pyrimidinyl-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

L23 ANSWER 33 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:431103 CAPLUS Full-text
DOCUMENT NUMBER: 115:31103
TITLE: Polyfunctional reactive dyes
INVENTOR(S): Herd, Karl Josef; Henk, Hermann; Stoehr, Frank Michael
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Eur. Pat. Appl., 105 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

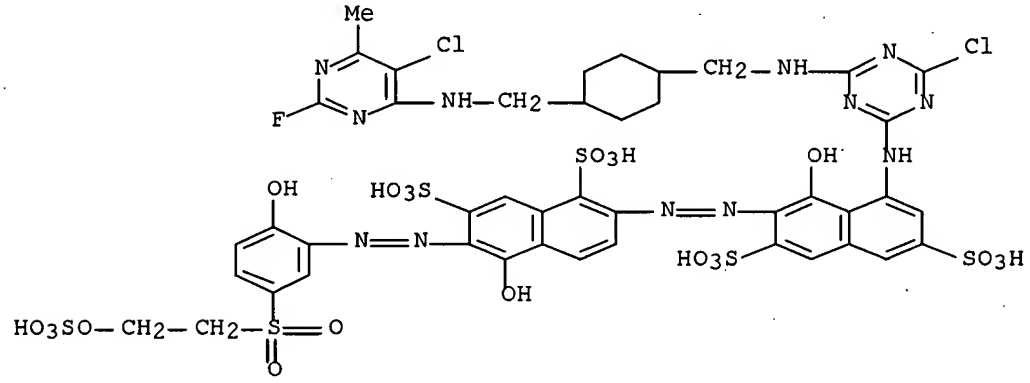
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 395951	A1	19901107	EP 1990-107503		19900420 <--
EP 395951	B1	19940824			
R: CH, DE, FR, GB, LI					
DE 3914628	A1	19901115	DE 1989-3914628		19890503 <--
JP 02308864	A	19901221	JP 1990-115335		19900502 <--
US 5274083	A	19931228	US 1991-724443		19910702 <--
PRIORITY APPLN. INFO.:			DE 1989-3914628	A	19890503 <--
			US 1990-511129	B1	19900419 <--

OTHER SOURCE(S): MARPAT 115:31103
ED Entered STN: 27 Jul 1991
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title dyes I [A = direct bond, divalent (cyclo)aliphatic bridging group, divalent aromatic aliphatic bridging group; D1, D2 = direct bond, divalent bridging group; G = chromophoric residue; R,R1,R2 = H, (un)substituted C1-4 alkyl; X = CH:CH2, CH2CH2Y; Y = alkyli-cleavable substituent; Y1 = F, Cl, Br; Z = fiber-reactive residue], useful for dyeing or printing hydroxyl or amide group-containing fabrics, are prepared Thus, 1-aminoethyl-3-sulfomethyl-4-methyl-6-hydroxy-2-pyridone was condensed with cyanuric chloride, the condensate condensed with ethylenediamine, 5-chloro-2,4,6-trifluoropyrimidine added, and the intermediate coupled with diazotized 2-amino-6-(β-sulfatoethylsulfonyl)-1- naphthalenesulfonic acid forming II which dyed cotton fabrics fast greenish yellow shades.
IT 134559-60-7
RL: USES (Uses)
(complexation of, with cupric sulfate)
RN 134559-60-7 CAPLUS
CN 1,7-Naphthalenedisulfonic acid, 2-[[8-[[4-chloro-6-[[[4-[[(5-chloro-2-

fluoro-6-methyl-4-pyrimidinyl)amino]methyl]cyclohexyl]methyl]amino]-1,3,5-triazin-2-yl]amino]-1-hydroxy-3,6-disulfo-2-naphthalenyl]azo]-5-hydroxy-6-[[2-hydroxy-5-[[2-(sulfooxy)ethyl]sulfonyl]phenyl]azo]- (9CI) (CA INDEX NAME)

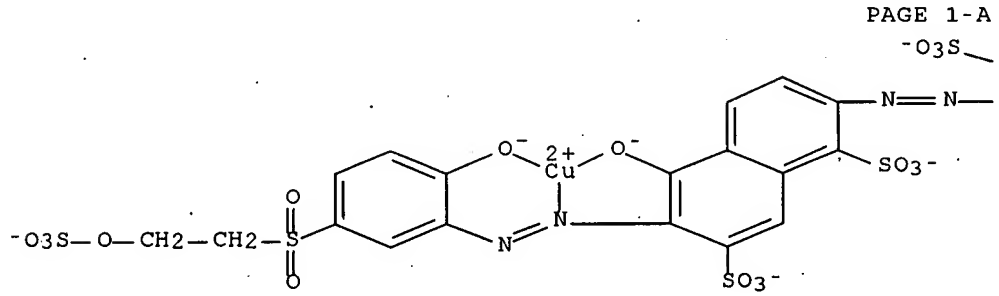


IT 134659-57-7P
RL: PREP (Preparation)
(manufacture of, as reactive dye)

RN 134659-57-7 CAPLUS

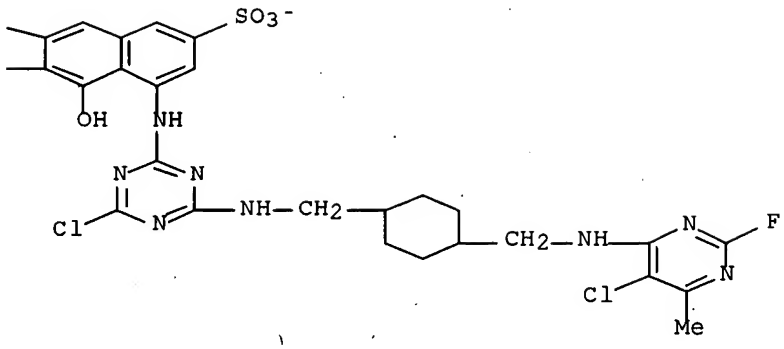
CN Cuprate(5-), [2-[[8-[[4-chloro-6-[[[4-[[(5-chloro-2-fluoro-6-methyl-4-pyrimidinyl)amino]methyl]cyclohexyl]methyl]amino]-1,3,5-triazin-2-yl]amino]-1-hydroxy-3,6-disulfo-2-naphthalenyl]azo]-5-hydroxy-6-[[2-hydroxy-5-[[2-(sulfooxy)ethyl]sulfonyl]phenyl]azo]-1,7-naphthalenedisulfonato(7-)]-, pentahydrogen (9CI) (CA INDEX NAME)

PAGE 1-A



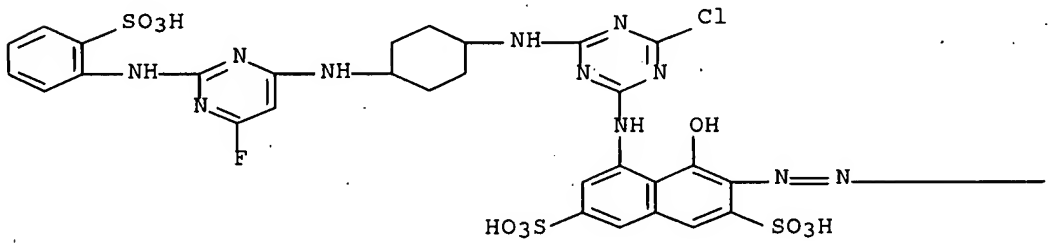
●5 H+

PAGE 1-B

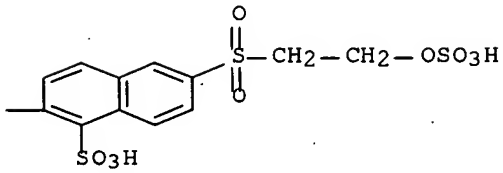


IT 134559-59-4P 134591-45-0P
RL: PREP (Preparation)
(manufacture of, as red reactive dye)
RN 134559-59-4 CAPLUS
CN 2,7-Naphthalenedisulfonic acid, 5-[[4-chloro-6-[[4-[[6-fluoro-2-[(2-sulfophenyl)amino]-4-pyrimidinyl]amino]cyclohexyl]amino]-1,3,5-triazin-2-yl]amino]-4-hydroxy-3-[[1-sulfo-6-[[2-(sulfooxy)ethyl]sulfonyl]-2-naphthalenyl]azo]- (9CI) (CA INDEX NAME)

PAGE 1-A

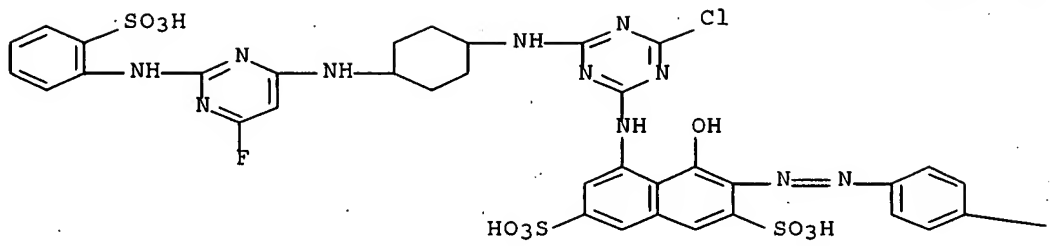


PAGE 1-B

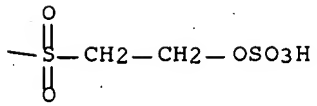


RN 134591-45-0 CAPLUS
CN 2,7-Naphthalenedisulfonic acid, 5-[[4-chloro-6-[[4-[[6-fluoro-2-[(2-sulfophenyl)amino]-4-pyrimidinyl]amino]cyclohexyl]amino]-1,3,5-triazin-2-yl]amino]-4-hydroxy-3-[[4-[[2-(sulfooxy)ethyl]sulfonyl]phenyl]azo]- (9CI) (CA INDEX NAME)

PAGE 1-A



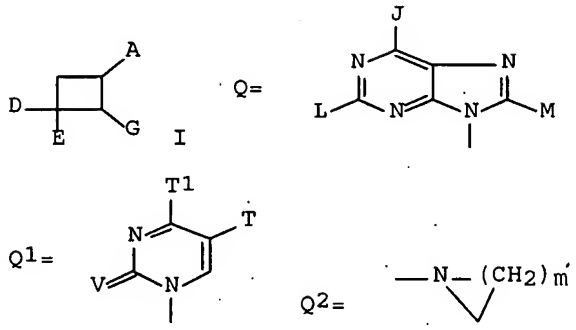
PAGE 1-B



L23 ANSWER 34 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1990:612577 CAPLUS Full-text
DOCUMENT NUMBER: 113:212577
TITLE: Preparation of nucleoside cyclobutane analogs as antiviral and antitumor agents
INVENTOR(S): Norbeck, Daniel W.; Plattner, Jacob J.; Rosen, Terry J.; Pariza, Richard J.; Sowin, Thomas J.; Garmaise, David L.; Hannick, Steven M.
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: Eur. Pat. Appl., 115 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 366059	A2	19900502	EP 1989-119703		19891024 <--
EP 366059	A3	19911218			
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE					
CA 2001318	A1	19900425	CA 1989-2001318		19891024 <--
DK 8905292	A	19900426	DK 1989-5292		19891024 <--
AU 8943785	A	19900503	AU 1989-43785		19891025 <--
JP 03047169	A	19910228	JP 1989-278337		19891025 <--
US 5153352	A	19921006	US 1990-570198		19900820 <--
US 5246931	A	19930921	US 1991-694538		19910501 <--
PRIORITY APPLN. INFO.:			US 1988-262547	A	19881025 <--
			US 1989-319385	A	19890303 <--
			US 1989-420691	A	19891017 <--

OTHER SOURCE(S): MARPAT 113:212577
ED Entered STN: 08 Dec 1990
GI

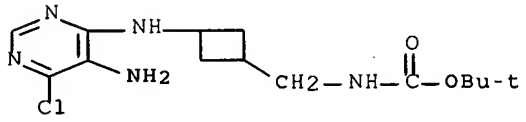


AB The title compds. [I; A = purin-9-yl (Q), pyrimidin-1-yl (Q1) or its heterocyclic isostere; J, L = H, OH, alkoxy, SH, thioalkoxy, N3, Q2, (un)substituted NH2, N:CHNH2, NHOH, or NHNH2; m = 1-6; M = H, alkyl, halo, Q2, (un)substituted NH2; T = H, alkyl, 2-haloethyl, halomethyl, CF2H, CF3, halo, cyano, NO2, CH:CH2, SH, NHOH, unsubstituted NH2, Q2, etc.; V = O, S; T1 = OH, SH, alkoxy, thioalkoxy, halo, Q2; D, G = H, alkyl, OH, CH2OH, alkoxymethyl, alkylcarbonyloxymethyl, aminoalkylcarbonyloxymethyl, etc.; E = H, CH2OH, OH;] are prepared Thus, condensation of 2,3- bis(hydroxymethyl)cyclobutylamine hydrochloride with 2-amino-4,6- dichlorpyrimidine in EtOH containing Et3N and diazo coupling of the resulting 3-[(2'-amino-6'-chloro-4'-pyrimidinyl)amino]-1,2- bis(hydroxymethyl)cyclobutane with 4-ClC6H4N2+Cl- followed by Zn reduction in AcOH gave 3-[(6'-chloro-2',5'-diamino-4'-pyrimidinyl)amino]-1,2-bis(hydroxymethyl)cyclobutane. Cyclocondensation of the latter with AcOCH2(OEt)2 under reflux followed by hydrolysis gave 9-[2',3'-bis(hydroxymethyl)cyclobutyl]guanine (II). Approx. 25 I were prepared and II in vitro was active against herpes simplex virus, human immunodeficiency virus 1 and 2, human cytomegalovirus, and Varicella-Zoster virus. II in vivo was active against hepatitis B virus in ducklings and HIV in mice. II and 4 other I showed antitumor activity against human lung carcinoma A549, human adenocarcinoma HCT-8 and mouse lymphocytic leukemia P388-DI.

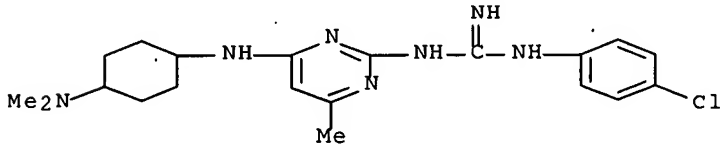
IT 130369-11-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for carbocyclic nucleoside cyclobutane analog)

RN 130369-11-8 CAPLUS

CN Carbamic acid, [[3-[(5-amino-6-chloro-4-pyrimidinyl)amino]cyclobutyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

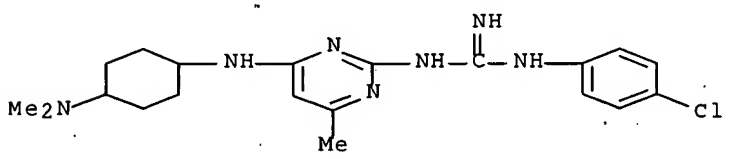


L23 ANSWER 35 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1980:34951 CAPLUS Full-text
DOCUMENT NUMBER: 92:34951
TITLE: Correlation analysis of pyrimidine folic acid antagonists as antibacterial agents. I
AUTHOR(S): Coats, Eugene A.; Genther, Clara S.; Smith, Carl C.
CORPORATE SOURCE: Coll. Pharm., Univ. Cincinnati, Cincinnati, OH, 45267, USA
SOURCE: European Journal of Medicinal Chemistry (1979), 14(3), 261-70
CODEN: EJMCA5; ISSN: 0009-4374
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
AB The activities of 175 pyrimidines as inhibitors of Streptococcus faecium, Lactobacillus casei, and Pediococcus cerevisiae are reported. In addition, the mode of action according to the ability of folic acid [59-30-3] or folinic acid [58-05-9] to reverse the inhibitory effect of the pyrimidines was determined The 2,4-diamino substituent pattern appeared to be the dominant but not the sole factor controlling mode of action. Quant. structure-activity relations using regression anal., substituent consts., and indicator variables were developed in an effort to delineate influences on potency and to quant. differences between the test systems. Although aromatic and(or) lipophilic substituents at the 5 position of 2,4-diaminopyrimidines enhanced folate reversible inhibition against all 3 systems the derived equations quant. establish differences in and limitations on the extent of this effect.
IT 51386-71-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(bactericidal activity of, structure in relation to)
RN 51386-71-1 CAPLUS
CN Guanidine, N-(4-chlorophenyl)-N'-[4-[[4-(dimethylamino)cyclohexyl]amino]-6-methyl-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

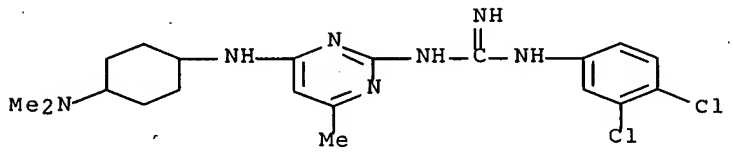


L23 ANSWER 36 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:103776 CAPLUS Full-text
DOCUMENT NUMBER: 80:103776
TITLE: Antimalarial drugs. 35. Synthesis and antimalarial effects of 1-(3,4-dichlorophenyl)-3-[4-[(1-ethyl-3-piperidyl)amino]-6-methyl-2-pyrimidinyl]guanidine and related substances
AUTHOR(S): Elslager, Edward F.; Werbel, Leslie M.; Curry, Ann; Headen, Nancy; Johnson, Judith
CORPORATE SOURCE: Res. Dev. Div., Parke, Davis and Co., Ann Arbor, MI, USA
SOURCE: Journal of Medicinal Chemistry (1974), 17(1), 75-100
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal

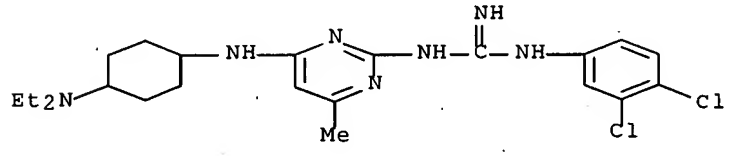
LANGUAGE: English
ED Entered STN: 12 May 1984
AB Structure-antimalarial activity of 1-(3,4-dichlorophenyl)-3-[4-[(1-ethyl-3-piperidyl)amino]-6-methyl-2-pyrimidinyl]guanidine (I) [21062-28-2] and 120 analogs prepared by condensation of the aryl(4-chloro-6-methyl-2-pyrimidinyl)guanidine derivs. with the appropriate polyamines is given. Curative activity against Plasmodium berghei infection in mice was shown by 90 compds. in single s.c. doses of 20-640 mg/kg. While 62 compds showed suppressive activity after oral administration, 46 of them were 2-30 times as potent as quinine-HCl [130-89-2]. Strong suppressive activity against P. gallinaceum in chicks was shown by 59 compds.
IT 51386-71-1P 51386-99-3P 51387-03-2P
51387-45-2P 51387-46-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and antimalarial activity of)
RN 51386-71-1 CAPLUS
CN Guanidine, N-(4-chlorophenyl)-N'-[4-[[4-(dimethylamino)cyclohexyl]amino]-6-methyl-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



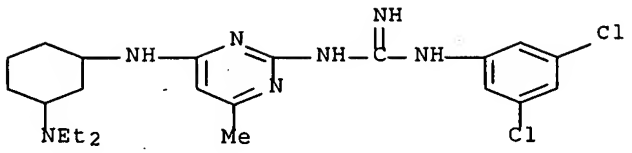
RN 51386-99-3 CAPLUS
CN Guanidine, N-(3,4-dichlorophenyl)-N'-[4-[[4-(dimethylamino)cyclohexyl]amino]-6-methyl-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 51387-03-2 CAPLUS
CN Guanidine, N-(3,4-dichlorophenyl)-N'-[4-[[4-(diethylamino)cyclohexyl]amino]-6-methyl-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 51387-45-2 CAPLUS
CN Guanidine, N-(3,5-dichlorophenyl)-N'-[4-[[3-(diethylamino)cyclohexyl]amino]-6-methyl-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 51387-46-3 CAPLUS
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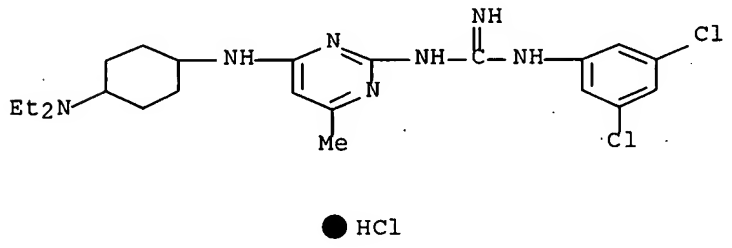
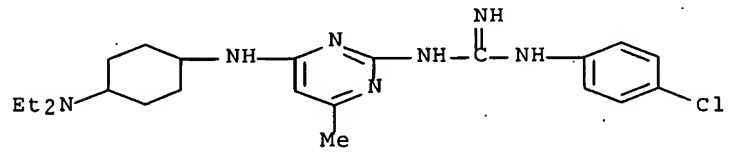
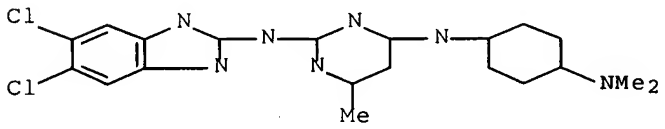


IT 51386-73-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 51386-73-3 CAPLUS
CN Guanidine, N-(4-chlorophenyl)-N'-[4-[[4-(diethylamino)cyclohexyl]amino]-6-methyl-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

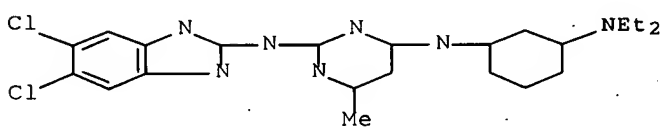


L23 ANSWER 37 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1973:478734 CAPLUS Full-text
DOCUMENT NUMBER: 79:78734
TITLE: Synthesis and antimalarial effects of 5,6-dichloro-2-[(4-[[4-(diethylamino)-1-methylbutyl]amino]-6-methyl-2-pyrimidinyl)amino]benzimidazole and related benzimidazoles and 1H-imidazo[4,5-b]pyridines
AUTHOR(S): Werbel, Leslie M.; Curry, Ann; Elslager, Edward F.; Hess, Carolyn
CORPORATE SOURCE: Res. Dev. Div., Parke, Davis and Co., Ann Arbor, MI, USA
SOURCE: Journal of Heterocyclic Chemistry (1973), 10(3), 363-82
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal

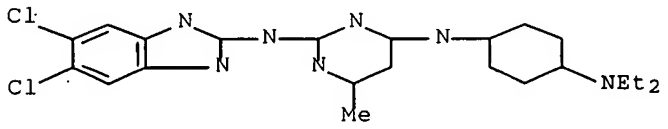
LANGUAGE: English
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB Fifty-five 2-[[4-[[(dialkylamino)alkyl]amino] - 6 - methyl - 2 - pyrimidinyl]amino]benzimidazoles were prepared in 3-88% yields by the condensation of the requisite 2-[(2-benzimidazolyl)amino]-4-chloro-6-methylpyrimidine with the appropriate polyamine in EtOH-HCl or neat with excess amine containing KI. The 2-[(2-benzimidazolyl)amino]-6-methyl-4-pyrimidinol precursors, obtained in 11-51% yields by cyclization of 2-(cyanoamino)-4-hydroxy-6-methylpyrimidine with a suitably substituted o-phenylenediamine, were chlorinated with POCl3 to give the intermediate 2-[(2-benzimidazolyl)amino]-4-chloro-6-methylpyrimidines (27-99%). Oxidation of 5,6-dichloro-2-[[4-[[4-(diethylamino)-1-methylbutyl]amino]-6-methyl-2-pyrimidinyl]amino]benzimidazole with m-chloroperbenzoic acid gave the distal N4'-oxide (19%). Fusion of 2,3-diaminopyridine with 2-(cyanoamino)-4-hydroxy-6-methylpyrimidine provided 2-[(4-hydroxy-6- methyl-2-pyrimidinyl)amino]-1H-imidazo[4,5-b]pyrimidine (30%), which upon chlorination with POCl3 (63%) followed by amination with N,N-diethylethylenediamine afforded 2-[4-[[2-(diethylamino)ethyl]amino]-6- methyl-2-pyrimidinyl]-1H-imidazo[4,5-b]pyridine (8%). Thirty-eight 2-[(4-amino-6-methyl-2-pyrimidinyl)amino]benzimidazoles possessed curvative activity against Plasmodium berghei at single subcutaneous doses ranging from 20-640 mg/kg. Orally, 31 compds. exhibited suppressive activity against P. berghei comparable with or superior to the reference drugs 1-(p-chlorophenyl)-3-[4-[[2-(diethylamino)ethyl]amino]-6-methyl-2-pyrimidinyl]guanidine (I) and quinine-HCl while 12 of them were 5 to 28 times as potent as I and quinine-HCl. Eight compds. also displayed strong suppressive activity against P. gallinaceum in chicks. 5,6-Dichloro-2-[[4-[2-(diethylamino)ethyl]amino]-6-methyl-2-pyrimidinyl]- benzimidazole showed marked activity against a cycloguanil-resistant line of P. berghei, and the most promising member of the series, i.e. 5,6-dichloro-2-[[4-[[4-(diethylamino)-1-methylbutyl]amino]-6-methyl-2-pyrimidinyl]amino]benzimidazole (I), was designated for preclinical toxicol. studies and clin. trial. Structure-activity relations are discussed.
IT 42388-86-3P 42388-91-0P 42388-92-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 42388-86-3 CAPLUS
CN 2,4-Pyrimidinediamine, N2-(5,6-dichloro-1H-benzimidazol-2-yl)-N4-[4-(dimethylamino)cyclohexyl]-6-methyl- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 42388-91-0 CAPLUS
CN 2,4-Pyrimidinediamine, N2-(5,6-dichloro-1H-benzimidazol-2-yl)-N4-[3-(diethylamino)cyclohexyl]-6-methyl- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 42388-92-1 CAPLUS
CN 2,4-Pyrimidinediamine, N2-(5,6-dichloro-1H-benzimidazol-2-yl)-N4-[4-(diethylamino)cyclohexyl]-6-methyl- (9CI) (CA INDEX NAME)

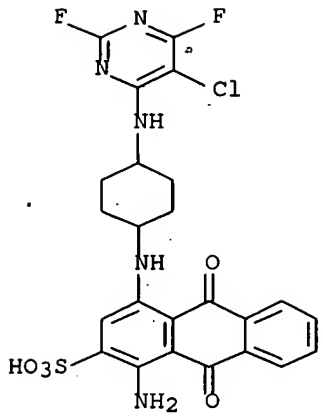


ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

L23 ANSWER 38 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1972:60924 CAPLUS Full-text
DOCUMENT NUMBER: 76:60924
TITLE: Fiber-reactive dyes
INVENTOR(S): Bien, Hans S.; Klauke, Erich
PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.
SOURCE: Brit. Amended, 75 pp.
CODEN: BSXXAH
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
GB 1169254	A	19700811	GB 1967-40774		19670906 <--
PRIORITY APPLN. INFO.:			DE 1966-F50181	A	19660910 <--
			DE 1967-F51942	A	19670325 <--

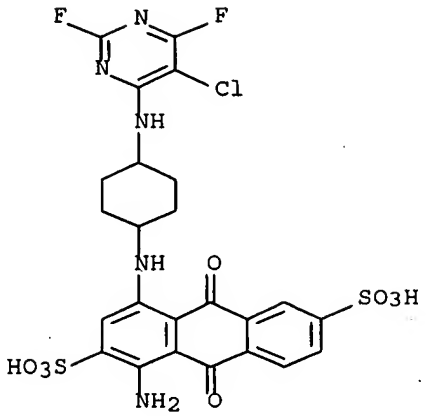
ED Entered STN: 12 May 1984
AB The title chlorodifluoropyrimidine dyes (I; R = H, Me; Q = anthraquinone, azo, metal complex azo, nitro, or Cu phthalocyanine dye residue), useful for dyeing cellulose and wool wetfast shades, were prepared by treating amino dyes with 5-chloro-2,4,6-trifluoropyrimidine (II). For example, diazotized 2-aminonaphthalene-4,8-disulfonic acid was coupled with m-toluidine, the azo dye dissolved in water, Me2CO and NaOH added, and the mixture treated with II at 20-30.deg. and pH 5.5-6 to give 2-[4-(5-chloro-2,6-difluoro-4-pyrimidinylamino)-o-tolylazo]naphthalene-4,8- disulfonic acid [34086-94-7], printing cellulose fabric wash- and lightfast reddish yellow. Similarly, 65 other I were prepared
IT 35434-62-9P
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)
RN 35434-62-9 CAPLUS
CN 2-Anthracenesulfonic acid, 1-amino-4-[[4-[(5-chloro-2,6-difluoro-4-pyrimidinyl)amino]cyclohexyl]amino]-9,10-dihydro-9,10-dioxo- (9CI) (CA INDEX NAME)



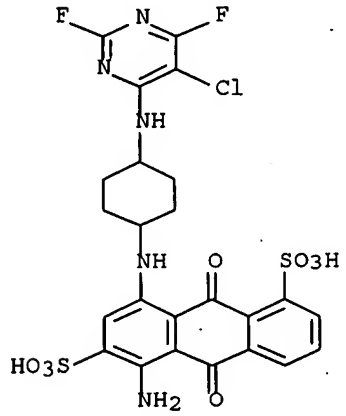
L23 ANSWER 39 OF 39 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1970:68209 CAPLUS Full-text
DOCUMENT NUMBER: 72:68209
TITLE: Fiber-reactive dyes
INVENTOR(S): Bien, Hans S.; Oertzen, Klaus V.; Harms, Wolfgang
PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.
SOURCE: Brit., 9 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1170195		19691112	GB 1968-10879	19680306 <--
DE 1644614			DE	
PRIORITY APPLN. INFO.:			DE	19670325 <--

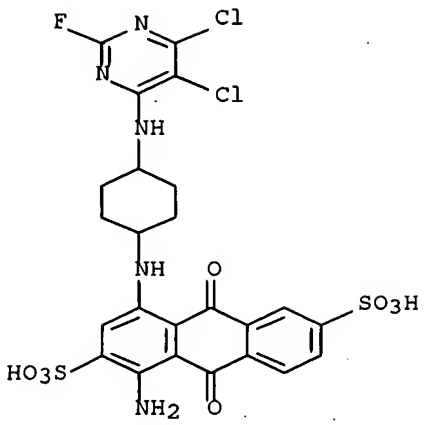
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB Compds. of the general formula I dye wool and cotton blue. Thus, 10.8 parts 1-amino-4-(4-aminocyclohexylamino)anthraquinone-2,6-disulfonic acid dissolved in 115 parts H2O was acylated at 0-5° with 3.7 parts 2,4,6-trifluoro-5-chloropyrimidine at pH 9-10, maintaining this pH with 2N NaOH, adjusted to pH 5.5 with HCl, and treated with 6 parts NaCl to precipitate I [R1 = R3 = H, R2 = SO3H, Y = Y1 (X = F)]. Similarly, other I were prepared (R1-R3 and Y given): H, SO3H, H, Y1 (X = Cl); H, SO3H, H, Y2 (Z = CO); H, SO3H, H, Y2 (Z = SO2); H, H, SO3H, Y1 (X = F); SO3H, H, H, Y1 (X = F).
IT 24460-66-0P 25980-28-3P 25980-29-4P
25980-32-9P
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)
RN 24460-66-0 CAPLUS
CN 2,6-Anthracenedisulfonic acid, 1-amino-4-[[4-[(5-chloro-2,6-difluoro-4-pyrimidinyl)amino]cyclohexyl]amino]-9,10-dihydro-9,10-dioxo- (8CI) (CA INDEX NAME)



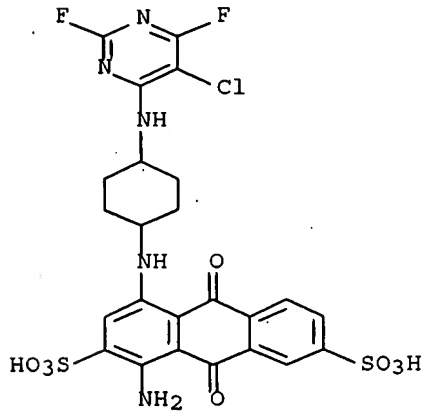
RN 25980-28-3 CAPLUS
CN 1,6-Anthracenedisulfonic acid, 5-amino-8-[[4-[(5-chloro-2,6-difluoro-4-pyrimidinyl)amino]cyclohexyl]amino]-9,10-dihydro-9,10-dioxo- (8CI) (CA INDEX NAME)



RN 25980-29-4 CAPLUS
CN 2,6-Anthracenedisulfonic acid, 1-amino-4-[[4-[(5,6-dichloro-2-fluoro-4-pyrimidinyl)amino]cyclohexyl]amino]-9,10-dihydro-9,10-dioxo- (8CI) (CA INDEX NAME)



RN 25980-32-9 CAPLUS
CN 2,7-Anthracenedisulfonic acid, 1-amino-4-[[4-[(5-chloro-2,6-difluoro-4-pyrimidinyl)amino]cyclohexyl]amino]-9,10-dihydro-9,10-dioxo- (8CI) (CA INDEX NAME)



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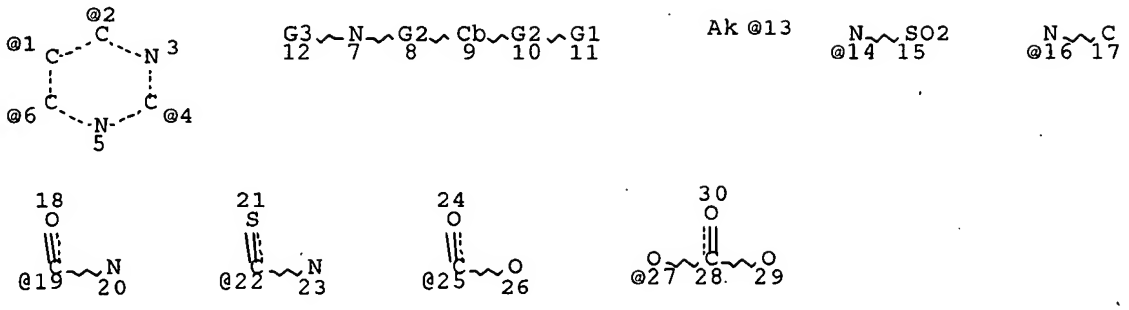

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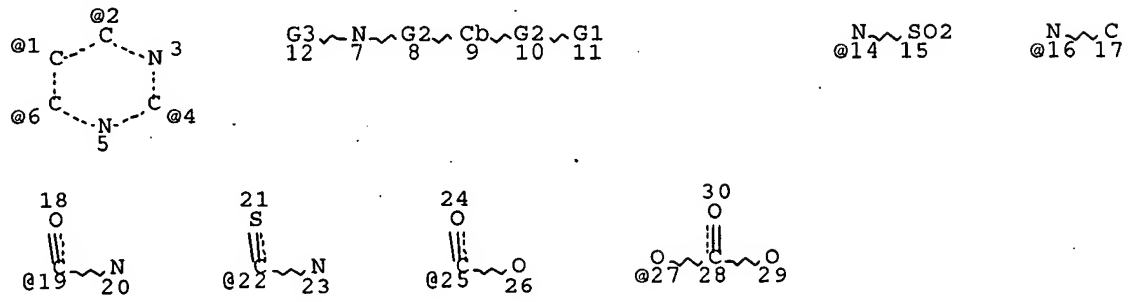

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DEFAULT ECLEVEL IS LIMITED

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ECOUNT  IS M4-X7 C  AT   9

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L9         563914 SEA ABB=ON  46.195.39/RID
L10           359 SEA ABB=ON  L9 AND L6

     FILE 'CAPLUS' ENTERED AT 09:36:01 ON 29 JUN 2007
L11             4 SEA ABB=ON  L10
L12             0 SEA ABB=ON  L11 AND (PY<2003 OR AY<2003 OR PRY<2003)

     FILE 'REGISTRY' ENTERED AT 09:37:04 ON 29 JUN 2007
L13        575386 SEA ABB=ON  DIMETHYLAMINO
L14           359 SEA ABB=ON  L10 AND L13
L15            13 SEA SUB=L9 SSS SAM L3
L16               STR L3
L17            13 SEA SUB=L9 SSS SAM (L16 AND L3)
                  D SCAN
L18        563914 SEA SUB=L9 SSS FUL (L16 AND L3) EXTEND
L19          3163 SEA SUB=L9 SSS FUL (L16 AND L3)
                  SAVE TEMP L19 JAI075FULL/A
L20           357 SEA ABB=ON  L19 AND L10
L21             2 SEA ABB=ON  L10 NOT L20
                  D SCAN

     FILE 'CAPLUS' ENTERED AT 09:43:11 ON 29 JUN 2007
L22            77 SEA ABB=ON  L19
L23            39 SEA ABB=ON  L22 AND (PY<2003 OR AY<2003 OR PRY<2003)
L24             0 SEA ABB=ON  L23 AND L5
L25             1 SEA ABB=ON  L22 AND L5

     FILE 'REGISTRY' ENTERED AT 09:44:18 ON 29 JUN 2007
                  D STAT QUE L19

     FILE 'CAPLUS' ENTERED AT 09:44:18 ON 29 JUN 2007
                  D QUE NOS L23
                  D IBIB ED ABS HITSTR L23 1-39

     FILE 'HOME' ENTERED AT 09:45:04 ON 29 JUN 2007
                  D STAT QUE L19

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